TABLE 1A



Table 2. Crystallographic data

| | Inflection, L1 | Peak, L2 | Remote, L3 | Native 1 | *Native 2 | *3'5'-ADP |
|---|----------------|-----------|------------|--------------|--------------|--------------|
| Data collection | 31 337 61 | 10 650 29 | 12 700 00 | 17 208 00 | | 12 308 00 |
| Energy, eV Wavelength 3. Å | 0.979537 | 0.979400 | 0.976259 | 1.00000 | 1.00000 | 1.00000 |
| Number of observations | 210,097 | 205,948 | 211,823 | 336,325 | 423,425 | 304,946 |
| Number of reflections | 54,462 | 55,080 | 54,821 | 59,335 | 126,451 | 162,841 |
| Number of unique reflections | 8,450 | 8,508 | 8,398 | 14,842 | 20,366 | 29,541 |
| Average redundancy | 6.4 | 6.5 | 6.5 | 4.0 | 6.2 | 5.5 |
| Completeness, % | | | | | | |
| All reflections | a95/90 | 92/88 | 94/88 | 96/84 | 64/86 | 100/99 |
| Reflections with I > 3a | 94/85 | 94/86 | 94/84 | 81/57 | 79/53 | 80/44 |
| <i u=""></i> | 40/14 | 41/19 | 40/18 | 25.6/4.5 | 26.5/3.0 | 31.1/3.8 |
| *Rueroe , % | 5.6/9.2 | 5.2/8.8 | 4.7/8.4 | 4.9/23.0 | 6.0/30.1 | 5.3/26.8 |
| Resolution, A | 2.8 | 2.8 | 2.8 | 2.4 | 2.0 | 1.9 |
| Refinement | | | | | | |
| Protein/Water | | | | 2,696/128 | 2,730/125 | 2,711/717,2 |
| Deviation form ideal geometry | | | | | | |
| bond length, Å / bond angles, ° | | | | 0.007/1.169 | 0.005/1.057 | 0.010/1.146 |
| dihedrals / imprpers, ° | | | | 25.956/0.588 | 23.123/0.610 | 22.247/0.770 |
| Ramachandran plot statistics Residues in most favorite / allowed regions, % | gions, % | | | 92.0/8.0 | 91.2/9.0 | 92.4/7.6 |
| †Rwork/Rfree, % | | | | 23.6/29.3 | 20.8/24.7 | 24.1/27.1 |

aData after slash sign correspond to outer shell

* $R_{merge} = \Sigma |I - \langle P \rangle / \Sigma I$, where I is the intensity of an individual measurement, and $\langle I \rangle$ is the mean intensity of this reflection

¹R_{free} is the cross-validation R-value calculated for 5% of the reflections omitted from the refinement.

 $\dagger R_{work} = \Sigma |F_o - F_c| / \Sigma |F_o|$, where $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes respectively.

*Space group for these data sets is monoclinic C2, the rest of the data sets belong to orthorombic P2,2,2 space group. Both of them contain one homotrimer per the asymmetric unit

TABLE 3

```
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 2.40 A
REMARK starting r= 0.2339 free r= 0.2899
REMARK final r= 0.2336 free_r= 0.2950
REMARK B rmsd for bonded mainchain atoms= 0.775 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 0.798 target= 2.0 REMARK B rmsd for angle mainchain atoms= 1.417 target= 2.0 REMARK B rmsd for angle sidechain atoms= 1.333 target= 2.5
REMARK wa= 3.19192
REMARK rweight=0.44902
REMARK target= mlf steps= 30
REMARK sg= P2(1)2(1)2(1) a= 49.824 b= 59.561 c= 113.738 alpha= 90 beta= 90
gamma= 90
REMARK parameter file 1 : CNX_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNX_TOPPAR:water_rep.param
REMARK parameter file 3 : CNX_TOPPAR:ion.param
REMARK parameter file 4 : so4/so4.param
REMARK molecular structure file: generate.psf
REMARK input coordinates: minimize.pdb
REMARK reflection file= x-ray data.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.40
REMARK initial B-factor correction applied to fobs :
REMARK B11= 5.613 B22= 4.955 B33= -10.569
         B12= 0.000 B13= 0.000 B23= 0.000
REMARK
REMARK B-factor correction applied to coordinate array B: 0.171
REMARK bulk solvent: (Mask) density level= 0.356315 e/A^3, B-factor= 44.7059 A^2
REMARK reflections with |Fobs|/sigma F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range:
                                                                          13818 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):
                                                                          537 (
                                                                                    3.9 % }
                                                                              0 (
                                                                                      0.0 % )
REMARK number of reflections rejected:
REMARK total number of reflections used:
                                                                          13281 ( 96.1 % )
REMARK number of reflections in working set:
                                                                          12603 ( 91.2 % )
                                                                             678 (
                                                                                     4.9 %)
REMARK number of reflections in test set:
REMARK FILENAME="acps native 1.pdb"/
REMARK Written by CNX VERSION:2000
           1 CB MET A1003 6.910 33.184 39.062 1.00 31.51
ATOM
           2 CG MET A1003
                                       5.553 33.663 38.598 1.00 33.32
ATOM
ATOM
           3 SD MET A1003
                                       4.818 34.801 39.816 1.00 36.27
                                      5.820 36.290 39.557 1.00 35.34

7.655 32.931 36.686 1.00 29.56

8.286 33.972 36.449 1.00 29.16

9.076 32.131 38.552 1.00 30.78

7.675 32.305 38.074 1.00 30.32
           4 CE MET A1003
ATOM
           5 C MET A1003
6 O MET A1003
7 N MET A1003
ATOM
                                                                                            0
MOTA
MOTA
           8 CA MET A1003
ATOM
           9 N ILE A1004
                                       6.935 32.292 35.768 1.00 28.43
ATOM
                                       6.826 32.791 34.401 1.00 27.65
MOTA
           10 CA ILE A1004
                                       6.307 31.701 33.452 1.00 28.01
6.103 32.287 32.051 1.00 27.49
7.294 30.525 33.430 1.00 27.59
6.890 29.404 32.482 1.00 28.22
5.885 33.992 34.322 1.00 26.94
           11 CB ILE A1004
MOTA
           12 CG2 ILE A1004
ATOM
           13 CG1 ILE A1004
MOTA
           14 CD1 ILE A1004
MOTA
           15 C
                    ILE A1004
MOTA
          16 0
MOTA
                    ILE A1004
                                      4.741 33.920 34.765 1.00 26.43
                                      6.380 35.088 33.750 1.00 25.94
           17 N VAL A1005
ATOM
                                                                                             С
           18 CA VAL A1005
                                       5.595 36.306 33.617 1.00 25.33
MOTA
           19 CB VAL A1005
                                        6.211 37.446 34.445 1.00 25.03
ATOM
```

| n mon | ~~ | 001 | | 21005 | c 200 | 36 005 | 25 000 | 1 00 05 00 | _ |
|-------|----|--------|-----|----------------|--------|------------------|------------------|------------|-----|
| ATOM | 20 | | | A1005 | 6.389 | 36.995 | 35.882 | 1.00 25.00 | C |
| ATOM | 21 | | | A1005 | 7.535 | 37.878 | 33.846 | 1.00 24.19 | С |
| ATOM | 22 | С | | A1005 | 5.432 | 36.796 | 32.173 | 1.00 25.45 | C |
| ATOM | 23 | 0 | VAL | A1005 | 4.982 | 37.920 | 31.949 | 1.00 25.63 | 0 |
| MOTA | 24 | N | GLY | A1006 | 5.794 | 35.964 | 31.197 | 1.00 25.11 | N |
| MOTA | 25 | CA | GLY | A1006 | 5.659 | 36.371 | 29.809 | 1.00 24.32 | C |
| ATOM | 26 | С | GLY | A1006 | 6.306 | 35.452 | 28.786 | 1.00 23.99 | С |
| ATOM | 27 | 0 | GLY | A1006 | 7.413 | 34.947 | 28.996 | 1.00 24.03 | 0 |
| ATOM | 28 | N | | A1007 | 5.613 | 35.232 | 27.671 | 1.00 23.11 | N |
| ATOM | 29 | CA | | A1007 | 6.132 | 34.386 | 26.603 | 1.00 22.22 | C |
| ATOM | 30 | СВ | | A1007 | 5.633 | 32.943 | 26.789 | 1.00 22.37 | C |
| ATOM | 31 | CG | | A1007 | 6.046 | 32.010 | 25.693 | 1.00 22.55 | Č |
| ATOM | 32 | | | A1007 | 5.331 | 31.123 | 24.961 | 1.00 22.89 | |
| ATOM | 33 | | | A1007 | 7.342 | 31.933 | 25.226 | 1.00 22.71 | N |
| ATOM | 34 | | | A1007 | 7.405 | 31.044 | 24.251 | 1.00 22.72 | |
| | | | | | | | | | • |
| ATOM | 35 | | | A1007 | 6.198 | 30.537 | 24.070 | 1.00 22.98 | N |
| ATOM | 36 | С | | A1007 | 5.718 | 34.925 | 25.234 | 1.00 21.79 | |
| ATOM | 37 | 0 | | A1007 | 4.553 | 35.230 | 25.007 | 1.00 21.69 | |
| ATOM | 38 | N | | A1008 | 6.682 | 35.054 | 24.325 | 1.00 21.62 | |
| ATOM | 39 | CA | | A1008 | 6.380 | 35.549 | 22.994 | 1.00 20.43 | |
| ATOM | 40 | С | GLY | A1008 | 7.237 | 34.888 | 21.932 | 1.00 20.87 | С |
| MOTA | 41 | 0 | GLY | A1008 | 8.396 | 34.554 | 22.171 | 1.00 20.58 | 0 |
| ATOM | 42 | N | ILE | A1009 | 6.655 | 34.663 | 20.760 | 1.00 20.92 | |
| MOTA | 43 | CA | ILE | A1009 | 7.389 | 34.077 | 19.652 | 1.00 21.06 | C |
| ATOM | 44 | CB | ILE | A1009 | 6.911 | 32.638 | 19.304 | 1.00 21.27 | C |
| ATOM | 45 | CG2 | ILE | A1009 | 7.140 | 31.699 | 20.485 | 1.00 21.48 | C |
| ATOM | 46 | CG1 | ILE | A1009 | 5.438 | 32.654 | 18.892 | 1.00 21.01 | С |
| ATOM | 47 | CD1 | ILE | A1009 | 4.967 | 31.340 | 18.285 | 1.00 20.98 | C |
| ATOM | 48 | С | ILE | A1009 | 7.184 | 34.951 | 18.420 | 1.00 21.74 | С |
| ATOM | 49 | 0 | | A1009 | 6.345 | 35.846 | 18.404 | 1.00 20.69 | |
| ATOM | 50 | N | | A1010 | 7.971 | 34.687 | 17.388 | 1.00 22.85 | |
| ATOM | 51 | CA | | A1010 | 7.857 | 35.416 | 16.147 | 1.00 23.91 | |
| ATOM | 52 | CB | | A1010 | 8.456 | 36.813 | 16.273 | 1.00 23.93 | |
| ATOM | 53 | CG | | A1010 | 8.300 | 37.622 | 14.998 | 1.00 24.40 | |
| ATOM | 54 | | | A1010 | 9.104 | 37.423 | 14.050 | 1.00 24.86 | |
| ATOM | 55 | | | A1010 | 7.357 | 38.442 | 14.030 | 1.00 24.36 | |
| | 56 | | | | 8.553 | | | 1.00 24.83 | |
| ATOM | 57 | С 0 | | A1010 A1010 | 9.586 | 34.658 34.037 | 15.041 15.262 | 1.00 24.83 | |
| ATOM | | | | | | | | | |
| ATOM | 58 | N | | A1011 | 7.959 | 34.687 | 13.852 | 1.00 25.82 | |
| ATOM | 59 | CA | | A1011 | 8.541 | 34.021 | 12.697 | 1.00 27.04 | |
| ATOM | 60 | CB | | A1011 | 7.713 | 32.780 | 12.258 | 1.00 26.91 | |
| ATOM | 61 | | | A1011 | 6.274 | 33.168 | 11.940 | 1.00 26.65 | |
| ATOM | 62 | | | A1011 | 8.378 | 32.126 | 11.048 | 1.00 27.05 | |
| ATOM | 63 | | | A1011 | 7.818 | 30.757 | 10.708 | 1.00 27.44 | |
| ATOM | 64 | С | | A1011 | 8.586 | 35.051 | 11.580 | 1.00 27.96 | |
| ATOM | 65 | 0 | | A1011 | 7.652 | 35.832 | 11.404 | 1.00 28.18 | |
| ATOM | 66 | N | | A1012 | 9.688 | 35.070 | 10.845 | 1.00 28.86 | |
| ATOM | 67 | CA | | A1012 | 9.841 | 36.023 | 9.762 | 1.00 30.03 | |
| MOTA | 68 | CB | | A1012 | 10.772 | 37.161 | 10.186 | 1.00 31.54 | |
| MOTA | 69 | CG | | A1012 | 10.071 | 38.292 | 10.895 | 1.00 33.83 | |
| ATOM | 70 | CD | | A1012 | 9,006 | 38.913 | 10.026 | 1.00 35.22 | |
| ATOM | 71 | | | A1012 | 9.352 | 39.404 | 8.927 | 1.00 36.13 | |
| ATOM | 72 | OE2 | | A1012 | 7.825 | 38.903 | 10.438 | 1.00 36.10 | |
| ATOM | 73 | С | GLU | A1012 | 10.375 | 35.414 | 8.487 | 1.00 29.94 | |
| ATOM | 74 | 0 | GLU | A1012 | 11.219 | 34.526 | 8.513 | 1.00 29.44 | 0 |
| ATOM | 75 | N | GLU | A1013 | 9.864 | 35.901 | 7.367 | 1.00 30.50 | |
| ATOM | 76 | CA | GLU | A1013 | 10.331 | 35.444 | 6.069 | 1.00 30.96 | 5 C |
| | | | | | | | | | |

| | | | | | | | | • | | |
|------|-----|-----|-----|---------|--------|--------|--------|------------|-----|---|
| ATOM | 77 | CB | GLU | A1013 | 9.236 | 35.587 | 5.012 | 1.00 31.74 | С | |
| ATOM | 78 | CG | GLU | A1013 | 9.629 | 34.951 | 3.693 | 1.00 33.86 | С | |
| ATOM | 79 | CD | GLU | A1013 | 8.621 | 35.179 | 2.582 | 1.00 35.01 | С | |
| ATOM | 80 | | | A1013 | 8.792 | 34.550 | 1.515 | 1.00 36.28 | 0 | |
| ATOM | 81 | | | A1013 | 7.675 | 35.980 | 2.762 | 1.00 35.21 | 0 | |
| ATOM | 82 | C | | A1013 | 11.498 | 36.372 | 5.735 | 1.00 30.42 | С | |
| | | | | | 11.348 | 37.594 | 5.750 | 1.00 30.06 | Ō | |
| ATOM | 83 | 0 | | A1013 | | 35.800 | 5.457 | 1.00 30.14 | N | |
| ATOM | 84 | N | | A1014 | 12.662 | | | 1.00 30.14 | . C | |
| ATOM | 85 | CA | | A1014 | 13.824 | 36.617 | 5.140 | | C | |
| MOTA | 86 | CB | | A1014 | 15.022 | 35.722 | 4.814 | 1.00 30.23 | | |
| ATOM | 87 | CG | LEU | A1014 | 15.552 | 34.904 | 6.000 | 1.00 30.34 | C | |
| MOTA | 88 | CD1 | LEU | A1014 | 16.618 | 33.929 | 5.533 | 1.00 30.59 | C | |
| MOTA | 89 | CD2 | LEU | A1014 | 16.117 | 35.835 | 7.053 | 1.00 30.41 | С | |
| ATOM | 90 | С | LEU | A1014 | 13.526 | 37.563 | 3.977 | 1.00 30.65 | С | |
| ATOM | 91 | 0 | LEU | A1014 | 13.877 | 38.743 | 4.023 | 1.00 30.37 | 0 | |
| ATOM | 92 | N | | A1015 | 12.857 | 37.048 | 2.949 | 1.00 30.96 | N | |
| ATOM | 93 | CA | | A1015 | 12.519 | 37.855 | 1.784 | 1.00 31.57 | С | |
| ATOM | 94 | CB | | A1015 | 11.683 | 37.038 | 0.798 | 1.00 30.98 | С | |
| ATOM | 95 | C | | A1015 | 11.780 | 39.131 | 2.183 | 1.00 31.93 | С | |
| | | | | | 11.947 | 40.170 | 1.544 | 1.00 31.75 | 0 | |
| ATOM | 96 | 0 | | A1015 | | 39.055 | 3.240 | 1.00 32.40 | N | |
| MOTA | 97 | N | | A1016 | 10.972 | 40.224 | | 1.00 32.40 | C | |
| ATOM | 98 | CA | | A1016 | 10.227 | | 3.714 | | C | |
| ATOM | 99 | CB | | A1016 | 9.264 | 39.844 | 4.847 | 1.00 33.61 | | |
| MOTA | 100 | OG | | A1016 | 8.316 | 38.883 | 4.428 | 1.00 34.88 | . 0 | |
| MOTA | 101 | С | | A1016 | 11.194 | 41.279 | 4.235 | 1.00 33.73 | С | |
| ATOM | 102 | 0 | SER | A1016 | 11.059 | 42.464 | 3.937 | 1.00 33.37 | 0 | |
| ATOM | 103 | N | ILE | A1017 · | 12.156 | 40.828 | 5.035 | 1.00 34.48 | . N | |
| MOTA | 104 | CA | ILE | A1017 | 13.167 | 41.698 | 5.615 | 1.00 35.17 | C | |
| ATOM | 105 | CB | ILE | A1017 | 14.041 | 40.922 | 6.641 | 1.00 34.97 | C | |
| ATOM | 106 | CG2 | ILE | A1017 | 15.151 | 41.814 | 7.173 | 1.00 34.62 | C | |
| ATOM | 107 | | | A1017 | 13.172 | 40.436 | 7.805 | 1.00 35.03 | С | |
| ATOM | 108 | | | A1017 | 12.550 | 41.555 | 8.623 | 1.00 34.83 | С | |
| ATOM | 109 | C | | A1017 | 14.064 | 42.266 | 4.516 | 1.00 35.70 | С | |
| ATOM | 110 | o | | A1017 | 14.435 | 43.439 | 4.555 | 1.00 35.49 | 0 | |
| ATOM | 111 | N | | A1018 | 14.414 | 41.431 | 3.542 | 1.00 36.59 | N | |
| | 112 | CA | | A1018 | 15.260 | 41.872 | 2.439 | 1.00 38.02 | C | |
| MOTA | | | | A1018 | 15.595 | 40.703 | 1.508 | 1.00 39.36 | c | |
| ATOM | 113 | CB | | | 16.768 | 40.703 | 0.578 | 1.00 42.30 | c | |
| ATOM | 114 | CG | | A1018 | | | -0.532 | 1.00 42.30 | c | |
| ATOM | 115 | CD | | A1018 | 16.928 | 39.967 | | 1.00 44.13 | o | |
| ATOM | 116 | OE1 | | A1018 | 16.923 | 38.748 | -0.239 | | 0 | |
| MOTA | 117 | | | A1018 | 17.069 | 40.387 | -1.703 | 1.00 45.34 | | |
| MOTA | 118 | С | | A1018 | 14.480 | 42.925 | 1.658 | 1.00 38.06 | C | |
| ATOM | 119 | 0 | | A1018 | 15.026 | 43.936 | 1.212 | 1.00 37.81 | 0 | |
| ATOM | 120 | N | SER | A1019 | 13.187 | 42.668 | 1.509 | 1.00 37.94 | N | |
| MOTA | 121 | CA | | A1019 | 12.297 | 43.561 | 0.799 | 1.00 37.74 | C | |
| ATOM | 122 | CB | SER | A1019 | 10.921 | 42.906 | 0.680 | 1.00 37.89 | C | |
| ATOM | 123 | OG | SER | A1019 | 9.994 | 43.764 | 0.044 | 1.00 38.96 | С | |
| MOTA | 124 | С | SER | A1019 | 12.182 | 44.916 | 1.505 | 1.00 37.72 | C | |
| ATOM | 125 | 0 | SER | A1019 | 12.074 | 45.957 | 0.850 | 1.00 37.89 | C |) |
| ATOM | 126 | N | ALA | A1020 | 12.207 | 44.902 | 2.836 | 1.00 37.14 | N | |
| ATOM | 127 | CA | | A1020 | 12.097 | 46.129 | 3.615 | 1.00 37.01 | C | 2 |
| ATOM | 128 | СВ | | A1020 | 11.773 | 45.800 | 5.063 | 1.00 36.69 | C | |
| ATOM | 129 | C | | A1020 | 13.369 | 46.973 | 3.542 | 1.00 37.03 | C | |
| ATOM | 130 | ŏ | | A1020 | 13.309 | 48.201 | 3.538 | 1.00 36.27 | | |
| ATOM | 131 | N | | A1021 | 14.519 | 46.309 | 3.497 | 1.00 37.47 | N | |
| ATOM | 132 | CA | | A1021 | 15.797 | 47.007 | 3.415 | 1.00 38.34 | | |
| | 133 | CB | | A1021 | 16.979 | | 3.651 | 1.00 37.99 | | 2 |
| MOTA | 133 | CD | VML | N WTOST | 10.313 | 40.04/ | 5.051 | 1.00 31.33 | ` | - |

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| ATOM | 134 | CG1 | VAL | A1021 | 18.282 | 46.740 | 3.316 | 1.00 38.47 | | С |
|--------------|------------|-----------|-----|----------------|------------------|------------------|----------------|--------------------------|---|--------|
| ATOM | 135 | CG2 | VAL | A1021 | 16.990 | 45.585 | 5.093 | 1.00 38.14 | | С |
| ATOM | 136 | | | A1021 | 15.937 | 47.605 | 2.025 | 1.00 38.86 | | С |
| ATOM | 137 | | | A1021 | 16.345 | 48.749 | 1.855 | 1.00 38.89 | • | 0 |
| ATOM | 138 | N | | A1022 | 15.586 | 46.810 | 1.029 | 1.00 39.74 | | N |
| ATOM | 139 | CA | | A1022 | 15.670 | 47.244 | -0.350 | 1.00 40.51 | | С |
| ATOM | 140 | | | A1022 | 15.220 | 46.117 | -1.300 | 1.00 40.54 | | С |
| ATOM | 141 | | | A1022 | 15.975 | 44.930 | -1.019 | 1.00 40.47 | | Ō |
| ATOM | 142 | | | A1022 | 15.442 | 46.525 | -2.753 | 1.00 41.07 | | Č |
| ATOM | 143 | | | A1022 | 14.795 | 48.472 | -0.579 | 1.00 40.85 | | Č |
| ATOM | 144 | Ö | | A1022 | 15.227 | 49.433 | -1.204 | 1.00 41.01 | • | Ö |
| ATOM | 145 | N | | A1023 | 13.577 | 48.442 | -0.048 | 1.00 41.28 | | N |
| ATOM | 146 | CA | | A1023 | 12.626 | 49.541 | -0.215 | 1.00 41.51 | | C |
| ATOM | 147 | | | A1023 | 11.198 | 49.003 | -0.083 | 1.00 41.55 | | Č |
| ATOM | 148 | CG | | A1023 | 10.804 | 48.042 | -1.201 | 1.00 42.10 | | Č |
| ATOM | 149 | CD | | A1023 | 9.460 | 47.375 | -0.938 | 1.00 42.16 | | Ċ |
| ATOM | 150 | | | A1023 | 8.439 | 48.328 | -0.514 | 0.05 42.12 | | N |
| ATOM | 151 | CZ | | A1023 | 7.158 | 48.021 | -0.344 | 0.05 42.14 | | C |
| ATOM | 152 | | | A1023 | 6.734 | 46.785 | -0.567 | 0.05 42.17 | | N |
| ATOM | 153 | | | A1023 | 6.300 | 48.947 | 0.061 | 0.05 42.16 | | N |
| ATOM | 154 | C | | A1023 | 12.798 | 50.747 | 0.710 | 1.00 41.61 | | C |
| | 155 | 0 | | A1023 | 12.796 | 51.851 | 0.363 | 1.00 41.34 | | Ô |
| ATOM | 156 | И | | A1023 | 13.395 | 50.544 | 1.878 | 1.00 41.34 | | N |
| ATOM | | | | A1024 | | 51.636 | 2.835 | 1.00 42.27 | | C |
| ATOM | 157 | CA | | | 13.583 | | 4.040 | 0.05 42.61 | | c |
| ATOM | 158 | CB | | A1024 | 12.658 | 51.445 | | | | C |
| ATOM | 159 | CG | | A1024 | 11.202 | 51.471 | 3.693 | 0.05 42.54 0.05 42.53 | | C |
| ATOM | 160 | | | A1024 | 10.233 | 50.537 | 3.841 | | | |
| ATOM | 161 | | | A1024 | 10.592 | 52.567 | 3.121 | 0.05 42.51 | | И С |
| ATOM | 162 | | | A1024 | 9.311 | 52.307 | 2.932 | 0.05 42.49 | | N |
| ATOM | 163 | | | A1024 | 9.067 | 51.081 | 3.360 | 0.05 42.48 1.00 43.14 | | C |
| ATOM | 164 | C | | A1024 A1024 | 15.028 | 51.727 | 3.307 4.131 | 1.00 43.14 | | 0 |
| MOTA | 165 | 0 | | | 15.483 | 50.930 | 2.782 | 1.00 43.24 | | N |
| MOTA | 166 | N | | A1025 | 15.732 | 52.722 | | 1.00 43.74 | | C |
| ATOM | 167 | CA | | A1025 | 17.139 | 52.963 | 3.089 | 1.00 44.50 | | c |
| ATOM | 168 | CB | | A1025 | 17.596 | 54.249 54.230 | 2.393 | 1.00 45.87 | | c |
| ATOM | 169 | CG | | A1025 | 17.396 | 55.420 | 0.208 | 1.00 46.86 | | c |
| ATOM | 170 171 | CD OF1 | | A1025 A1025 | 18.031 19.267 | 55.571 | 0.320 | 1.00 47.25 | | Ö |
| ATOM | | | | | 17.294 | 56.201 | -0.434 | 1.00 47.23 | | ő |
| ATOM | 172 173 | C | | A1025 A1025 | 17.539 | 53.030 | 4.565 | 1.00 47.49 | | c |
| ATOM | 174 | 0 | | A1025 | 18.655 | 52.645 | 4.912 | 1.00 43.56 | | Õ |
| ATOM | 175 | | | A1025 | 16.649 | 53.523 | 5.424 | 1.00 42.64 | | N |
| ATOM ATOM | 176 | N CA | | A1026 | 16.972 | 53.631 | 6.838 | 1.00 41.75 | | Ĉ |
| ATOM | 177 | C | | A1026 | 16.244 | 52.645 | 7.731 | 1.00 41.40 | | Č |
| ATOM | 178 | 0 | | A1026 | 16.091 | 52.877 | | 1.00 41.35 | | Õ |
| ATOM | 179 | N | | A1027 | 15.801 | 51.537 | 7.144 | 1.00 40.74 | | N |
| ATOM | 180 | CA | | A1027 | 15.077 | 50.500 | 7.871 | 1.00 39.69 | | C |
| | 181 | CB | | A1027 | 14.695 | 49:376 | 6.906 | 1.00 33.03 | | Č |
| ATOM ATOM | 182 | CG | | A1027 | 13.976 | 48.233 | 7.558 | 1.00 40.05 | | c |
| | 183 | | | A1027 | 12.654 | 48.369 | 7.978 | 1.00 40.03 | | c |
| ATOM ATOM | 184 | | | A1027 | 14.618 | 47.012 | 7.748 | 1.00 40.03 | | c |
| ATOM | 185 | | | A1027 | 11.982 | 47.301 | 8.576 | 1.00 39.83 | | C |
| ATOM | 186 | | | A1027 | 13.955 | 45.944 | 8.344 | 1.00 39.33 | • | c |
| ATOM | 187 | CEZ | | A1027 | 12.636 | 46.089 | 8.757 | 1.00 39.71 | | c |
| ATOM | 188 | C | | A1027 | 15.900 | 49.920 | 9.020 | 1.00 39.08 | | c |
| ATOM | 189 | 0 | | A1027 | 15.470 | 49.929 | 10.175 | 1.00 39.00 | | o |
| ATOM | 190 | N | | A1027 | 17.080 | 49.409 | | 1.00 38.48 | | N |
| ATOM | 130 | IA | NIM | MIUZO | 17.000 | 49.403 | , 0.002 | 1.00 20.40 | | 14 |

| ATOM | 191 | CA | ALA | A1028 | 17.980 | 48.811 | 9.656 | 1.00 38.36 | С |
|--------------|------------|-----|-----|----------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 192 | CB | ALA | A1028 | 19.242 | 48.321 | 8.960 | 1.00 37.96 | С |
| ATOM | 193 | С | ALA | A1028 | 18.349 | 49.784 | 10.764 | 1.00 38.25 | С |
| ATOM | 194 | 0 | | A1028 | 18.533 | 49.384 | 11.907 | 1.00 38.15 | 0 |
| ATOM | 195 | N | LYS | A1029 | 18.456 | 51.061 | 10.418 | 1.00 38.38 | N |
| MOTA | 196 | CA | | A1029 | 18.823 | 52.094 | 11.380 | 1.00 38.44 | С |
| ATOM | 197 | CB. | | A1029 | 19.154 | 53.391 | 10.636 | 1.00 39.34 | . С |
| ATOM | 198 | CG | LYS | A1029 | 19.997 | 54.393 | 11.411 | 1.00 40.55 | С |
| ATOM | 199 | CD | LYS | A1029 | 19.248 | 55.005 | 12.591 | 1.00 41.77 | С |
| ATOM | 200 | CE | LYS | A1029 | 20.043 | 56.146 | 13.215 | 1.00 41.81 | С |
| ATOM | 201 | ΝZ | | A1029 | 20.282 | 57.218 | 12.208 | 1.00 42.20 | N |
| ATOM | 202 | С | | A1029 | 17.703 | 52.331 | 12.386 | 1.00 37.98 | С |
| ATOM | 203 | 0 | | A1029 | 17.948 | 52.731 | 13.522 | 1.00 38.26 | 0 |
| ATOM | 204 | N | | A1030 | 16.470 | 52.084 | 11,969 | 1.00 37.55 | N |
| MOTA | 205 | CA | | A1030 | 15.330 | 52.267 | 12.856 | 1.00 37.18 | C |
| ATOM | 206 | CB | | A1030 | 14.050 | 52.489 | | 1.00 38.15 | C |
| ATOM | 207 | CG | | A1030 | 13.833 | 53.934 | 11.573 | 1.00 39.87 | C |
| ATOM | 208 | CD | | A1030 | 12.449 | | 10.937 | 1.00 40.62 | C |
| ATOM | 209 | NE | | A1030 | 12.383 | 53.532 | 9.598 | 1.00 41.54 | N |
| ATOM | 210 | CZ | | A1030 | 12.825 | 54.142 | 8.500 | 1.00 42.11 | C |
| ATOM | 211 | | | A1030 | 13.359 | 55.355 | 8.577 | 1.00 41.94 | N |
| ATOM | 212 | | | A1030 | 12.747 | 53.533 | 7.323 | 1.00 42.66 | N C |
| ATOM | 213 | С | | A1030 | 15.145 | 51.064 | 13.780 | 1.00 36.44 | 0 |
| ATOM | 214 | 0 | | A1030 | 14.650 | 51.202 | 14.900 | 1.00 36.62 | N |
| ATOM | 215 | N | | A1031 | 15.560 | 49.889 | 13.313 | 1.00 35.30 1.00 34.12 | C |
| ATOM | 216 | CA | | A1031 A1031 | 15.417 | 48.655 | 14.080 13.145 | 1.00 34.12 | c |
| ATOM | 217 218 | CB | | | 15.160 14.965 | 47.458 46.190 | 13.143 | 1.00 34.23 | c |
| ATOM | | | | A1031 | | | 12.279 | 1.00 34.33 | c |
| ATOM | 219 | CGZ | | A1031 | 13.949 16.615 | 47.723 48.300 | 14.960 | 1.00 34.77 | C |
| ATOM ATOM | 220 221 | 0 | | A1031 A1031 | 16.447 | 47.763 | 16.057 | 1.00 33.18 | 0 |
| ATOM | 222 | Ŋ | | A1031 | 17.818 | 48.595 | 14.482 | 1.00 33.04 | N |
| ATOM | 223 | CA | | A1032 | 19.026 | 48.264 | 15.226 | 1.00 31.30 | Č |
| ATOM | 224 | CB | | A1032 | 20.081 | 47.692 | 14.274 | 1.00 30.83 | Č |
| ATOM | 225 | CG | | A1032 | 19.665 | 46.475 | 13.438 | 1.00 30.70 | Ċ |
| ATOM | 226 | | | A1032 | 20.852 | 46.007 | 12.608 | 1.00 30.16 | C |
| ATOM | 227 | | | A1032 | 19.172 | 45.351 | 14.349 | 1.00 30.17 | C |
| ATOM | 228 | C | | A1032 | 19.634 | 49.422 | 16.005 | 1.00 30.91 | C |
| ATOM | 229 | 0 | | A1032 | 19.534 | 50.578 | 15.602 | 1.00 31.10 | 0 |
| ATOM | 230 | N | | A1033 | 20.262 | 49.095 | 17.129 | 1.00 30.41 | N |
| MOTA | 231 | CA | THR | A1033 | 20.918 | 50.094 | 17.960 | 1.00 29.93 | С |
| ATOM | 232 | CB | | A1033 | 21.113 | 49.605 | 19.410 | 1.00 29.26 | С |
| ATOM | 233 | OG1 | THR | A1033 | 22.084 | 48.552 | 19.438 | 1.00 28.24 | 0 |
| ATOM | 234 | CG2 | THR | A1033 | 19.800 | 49.097 | 19.980 | 1.00 29.31 | С |
| ATOM | 235 | С | THR | A1033 | 22.291 | 50.334 | 17.339 | | С |
| ATOM | 236 | 0 | THR | A1033 | 22.678 | 49.633 | 16.405 | 1.00 29.45 | 0 |
| ATOM | 237 | N | ALA | A1034 | 23.018 | 51.321 | 17.856 | 1.00 30.49 | N |
| MOTA | 238 | CA | ALA | A1034 | 24.344 | 51:638 | 17.339 | 1.00 31.05 | С |
| ATOM | 239 | CB | ALA | A1034 | 24.987 | 52.734 | 18.177 | 1.00 30.92 | C |
| MOTA | 240 | С | ALA | A1034 | 25.211 | 50.388 | 17.356 | 1.00 31.28 | С |
| MOTA | 241 | 0 | | A1034 | 25.837 | 50.047 | 16.357 | 1.00 31.20 | 0 |
| ATOM | 242 | N | | A1035 | 25.241 | 49.706 | 18.495 | 1.00 31.90 | N |
| MOTA | 243 | CA | | A1035 | 26.030 | 48.487 | 18.619 | 1.00 32.66 | C |
| MOTA | 244 | CB | | A1035 | 25.878 | 47.907 | 20.031 | 1.00 32.74 | C |
| MOTA | 245 | CG | | A1035 | 26.464 | 48.733 | 21.195 | 1.00 32.90 | C |
| MOTA | 246 | | | A1035 | 26.003 | 48.158 | 22.529 | | C |
| ATOM | 247 | CD2 | LEU | A1035 | 27.985 | 48.737 | 21.121 | 1.00 32.56 | C |

| MOTA | 248 | С | LEU | A1035 | 25.612 | 47.454 | 17.556 | 1.00 33.36 | С |
|--------------|------------|----------|-----|----------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 249 | 0 | LEU | A1035 | 26.442 | 46.992 | 16.769 | 1.00 33.53 | 0 |
| ATOM | 250 | N | GLU | A1036 | 24.328 | 47.104 | 17.526 | 1.00 33.64 | N |
| ATOM | 251 | CA | | A1036 | 23.822 | 46.140 | 16.555 | 1.00 34.14 | С |
| ATOM | 252 | CB | GLU | A1036 | 22.299 | 46.014 | 16.682 | 1.00 33.87 | С |
| ATOM | 253 | CG | | A1036 | 21.818 | 45.217 | 17.890 | 1.00 33.65 | С |
| ATOM | 254 | CD | | A1036 | 20.341 | 45.462 | 18.216 | 1.00 33.37 | C |
| ATOM | 255 | | | A1036 | 19.726 | 44.613 | 18.895 | 1.00 32.88 | 0 |
| ATOM | 256 | | | A1036 | 19.797 | 46.509 | 17.808 | 1.00 33.01 | 0 |
| MOTA | 257 | С | | A1036 | 24.188 | 46.573 | 15.137 | 1.00 34.85 | C |
| MOTA | 258 | 0 | | A1036 | 24.526 | 45.752 | 14.284 | 1.00 34.59 | 0 |
| ATOM | 259 | N | | A1037 | 24.120 | 47.875 | 14.893 | 1.00 35.84 | N |
| ATOM | 260 | CA | | A1037 | 24.436 | 48.433 | 13.585 | 1.00 37.02 | С |
| ATOM | 261 | CB. | | A1037 | 24.172 | 49.936 | 13.605 | 1.00 37.11 | C |
| ATOM | 262 | CG | | A1037 | 23.656 | 50.510 | 12.294 | 1.00 38.16 | С |
| MOTA | 263 | SD | | A1037 | 22.148 | 49.717 | 11.685 | 1.00 38.53 | S |
| MOTA | 264 | CE | | A1037 | 22.507 | 49.661 | 9.949 | 1.00 38.71 | C |
| ATOM | 265 | С | | A1037 | 25.899 | 48.141 | 13.215 | 1.00 37.76 | C |
| MOTA | 266 | 0 | | A1037 | 26.227 | 47.928 | 12.044 | 1.00 37.71 | 0 |
| MOTA | 267 | N | | A1038 | 26.774 | 48.117 | 14.217 | 1.00 38.51 | N |
| MOTA | 268 | CA | | A1038 | 28.183 | 47.835 | 13.977 | 1.00 39.30 | C C |
| ATOM | 269 | CB | | A1038 | 28.989 | 47.966 | 15.275 | 1.00 40.38 | C |
| ATOM | 270 | CG | | A1038 | 28.963 | 49.369 49.513 | 15.880 | 1.00 41.32 1.00 42.00 | C |
| ATOM | 271 | CD | | A1038 | 29.874 | | 17.086 17.771 | 1.00 42.00 | 0 |
| MOTA | 272 | | | A1038 | 29.789 | 50.553 48.592 | 17.771 | 1.00 42.33 | 0 |
| ATOM | 273 | | | A1038 A1038 | 30.677 28.349 | 46.436 | 13.395 | 1.00 39.50 | c |
| ATOM | 274 | С | | | 28.932 | 46.430 | 12.327 | 1.00 40.05 | ō |
| ATOM | 275 | 0 | | A1038 A1039 | 27.837 | 45.423 | 14.087 | 1.00 39.36 | N |
| ATOM | 276 277 | N | | A1039 | 27.037 | 44.063 | 13.577 | 1.00 39.30 | c |
| MOTA MOTA | 278 | CA CB | | A1039 | 27.343 | 43.053 | 14.563 | 1.00 39.62 | Ċ |
| ATOM | 279 | CG | | A1039 | 27.395 | 41.632 | 14.025 | 1.00 40.25 | c |
| ATOM | 280 | CD | | A1039 | 27.177 | 40.585 | 15.089 | 1.00 40.85 | Č |
| ATOM | 281 | NE | | A1039 | 27.251 | 39.243 | 14.516 | 1.00 41.68 | N |
| ATOM | 282 | CZ | | A1039 | 28.314 | 38.756 | 13.879 | 1.00 42.00 | C |
| ATOM | 283 | | | A1039 | 28.289 | 37.523 | 13.387 | 1.00 42.01 | N |
| ATOM | 284 | | | A1039 | 29.408 | 39.496 | 13.735 | 1.00 41.92 | N |
| ATOM | 285 | C | | A1039 | 27.241 | 43.938 | 12.228 | 1.00 39.03 | С |
| ATOM | 286 | Ö | | A1039 | 27.774 | 43.347 | 11.291 | 1.00 38.64 | 0 |
| ATOM | 287 | N | | A1040 | 26.040 | 44.502 | 12.136 | 1.00 39.10 | N |
| ·ATOM | 288 | CA | | A1040 | 25.255 | 44.464 | 10.901 | 1.00 39.18 | С |
| ATOM | 289 | СВ | | A1040 | 24.030 | 45.369 | 11.036 | 1.00 38.05 | С |
| ATOM | 290 | CG | PHE | A1040 | 23.268 | 45.560 | 9.754 | 1.00 37.43 | С |
| ATOM | 291 | CD1 | PHE | A1040 | 22.443 | 44.557 | 9.258 | 1.00 37.16 | С |
| ATOM | 292 | CD2 | PHE | A1040 | 23.365 | 46.752 | 9.045 | 1.00 37.16 | С |
| ATOM | 293 | CE1 | PHE | A1040 | 21.722 | 44.742 | 8.074 | 1.00 36.76 | C |
| MOTA | 294 | CE2 | PHE | A1040 | 22.649 | 46.946 | 7.863 | 1.00 36.76 | С |
| ATOM | 295 | CZ | PHE | E A1040 | 21.825 | 45:936 | 7.379 | 1.00 36.61 | C |
| MOTA | 296 | С | PHE | E A1040 | 26.063 | 44.910 | 9.682 | 1.00 39.84 | C |
| MOTA | 297 | 0 | | E A1040 | 26.157 | 44.190 | 8.682 | 1.00 39.67 | 0 |
| MOTA | 298 | N | | R A1041 | 26.643 | 46.104 | 9.774 | 1.00 40.57 | N |
| ATOM | 299 | CA | | R A1041 | 27.415 | 46.668 | 8.676 | 1.00 41.24 | С |
| MOTA | 300 | CB | | R A1041 | 27.726 | 48.138 | 8.938 | 1.00 41.14 | C |
| MOTA | 301 | | | R A1041 | 28.364 | 48.272 | 10.212 | 1.00 41.93 | 0 |
| ATOM | 302 | | | R A1041 | 26.446 | 48.948 | 8.933 | 1.00 40.95 | C |
| ATOM | 303 | C | | R A1041 | 28.708 | 45.931 | 8.353 | 1.00 41.72 | С |
| ATOM | 304 | 0 | THE | R A1041 | 29.251 | 46.080 | 7.259 | 1.00 41.99 | 0 |

| ATOM | 305 | N | SER | A1042 | 29.198 | 45.133 | 9.297 | 1.00 42.15 | N |
|------|-------|-----|-----|-------|------------------|--------|--------|------------|-----|
| ATOM | 306 | CA | SER | A1042 | 30.419 | 44.367 | 9.078 | 1.00 42.65 | . ¢ |
| ATOM | 307 | СВ | SER | A1042 | 31.106 | 44.057 | 10.407 | 1.00 42.64 | C |
| ATOM | 308 | OG | SER | A1042 | 30.642 | 42.828 | 10.934 | 1.00 43.03 | 0 |
| ATOM | 309 | С | | A1042 | 30.066 | 43.050 | 8.381 | 1.00 43.22 | С |
| ATOM | 310 | 0 | | A1042 | 30.937 | 42.218 | 8.118 | 1.00 43.14 | 0 |
| ATOM | 311 | N | | A1043 | 28.781 | 42.869 | 8.095 | 1.00 43.80 | N |
| ATOM | 312 | | | A1043 | 28.298 | 41.660 | 7.439 | 1.00 44.32 | C |
| ATOM | 313 | CB | | A1043 | 27.151 | 41.040 | 8.247 | 1.00 43.98 | Č |
| ATOM | 314 | CG | | A1043 | 27.491 | 40.512 | 9.642 | 1.00 43.88 | c |
| ATOM | 315 | | | A1043 | 26.219 | 40.165 | 10.388 | 1.00 43.76 | C |
| | 316 | | | A1043 | 28.383 | 39.294 | 9.521 | 1.00 44.03 | C |
| ATOM | | | | A1043 | | | 6.026 | 1.00 44.03 | C |
| MOTA | 317 | | | | 27.821 27.448 | 41.973 | 5.722 | | 0 |
| ATOM | 318 | 0 | | A1043 | | 43.110 | | 1.00 44.88 | |
| ATOM | 319 | N | | A1044 | 27.827 | 40.950 | 5.174 | 1.00 45.38 | N |
| ATOM | 320 | CA | | A1044 | 27.412 | 41.088 | 3.782 | 1.00 45.95 | C |
| ATOM | 321 | CB | | A1044 | 28.556 | 40.673 | 2.856 | 1.00 46.91 | C |
| MOTA | 322 | CG | | A1044 | 28.976 | 39.209 | 3.060 | 1.00 47.97 | С |
| ATOM | 323 | CD | | A1044 | 29.803 | 38.669 | 1.896 | 1.00 48.98 | С |
| MOTA | 324 | CE | | A1044 | 30.319 | 37.260 | 2.187 | 1.00 49.35 | C |
| ATOM | 325 | NZ | | A1044 | 29.216 | 36.313 | 2.505 | 1.00 49.24 | N |
| ATOM | 326 | С | | A1044 | 26.202 | 40.217 | 3.457 | 1.00 45.75 | С |
| MOTA | 327 | 0 | | A1044 | 25.779 | 39.391 | 4.266 | 1.00 46.06 | 0 |
| MOTA | 328 | N | | A1045 | 25.674 | 40.416 | 2.252 | 1.00 45.39 | N |
| ATOM | 329 | CA | | A1045 | 24.538 | 39.663 | 1.743 | 1.00 44.96 | С |
| ATOM | 330 | С | GLY | A1045 | 23.577 | 38.960 | 2.685 | 1.00 44.52 | С |
| ATOM | 331 | 0 | GLY | A1045 | 23.147 | 39.520 | 3.692 | 1.00 44.43 | 0 |
| ATOM | 332 | N | ARG | A1046 | 23.231 | 37.726 | 2.333 | 1.00 44.21 | N |
| ATOM | 333 | CA | ARG | A1046 | 22.297 | 36.917 | 3.112 | 1.00 43.89 | С |
| ATOM | 334 | CB | ARG | A1046 | 22.304 | 35.474 | 2.589 | 1.00 44.58 | С |
| ATOM | 335 | CG | ARG | A1046 | 21.962 | 35.399 | 1.099 | 1.00 46.46 | С |
| ATOM | 336 | CD | ARG | A1046 | 21.891 | 33.977 | 0.547 | 1.00 47.97 | С |
| ATOM | 337 | NE | ARG | A1046 | 20.698 | 33.253 | 0.979 | 1.00 49.25 | N |
| ATOM | 338 | CZ | ARG | A1046 | 20.360 | 32.043 | 0.538 | 1.00 49.83 | С |
| ATOM | 339 | NH1 | ARG | A1046 | 19.257 | 31.454 | 0.983 | 1.00 49.98 | N |
| ATOM | 340 | NH2 | ARG | A1046 | 21.123 | 31.420 | -0.352 | 1.00 49.87 | N |
| MOTA | 341 | С | ARG | A1046 | 22.572 | 36.951 | 4.609 | 1.00 43.05 | С |
| ATOM | 342 | 0 | | A1046 | 21:657 | 37.167 | 5.402 | 1.00 42.92 | 0 |
| ATOM | 343 | N | ARG | A1047 | 23.830 | 36.751 | 4.994 | 1.00 42.04 | N |
| ATOM | 344 | CA | ARG | A1047 | 24.212 | 36.775 | 6.401 | 1.00 40.92 | С |
| ATOM | 345 | CB | ARG | A1047 | 25.726 | 36.592 | 6.553 | 1.00 41.86 | С |
| ATOM | 346 | CG | ARG | A1047 | 26.196 | 35.146 | 6.581 | 1.00 43.21 | С |
| ATOM | 347 | CD | | A1047 | 27.613 | 35.070 | 7.134 | 1.00 44.61 | С |
| MOTA | 348 | NE | | A1047 | 28.023 | 33.709 | 7.475 | 1.00 45.70 | N |
| ATOM | 349 | CZ | | A1047 | 28.346 | 32.773 | 6.588 | 1.00 46.26 | C |
| ATOM | 350 | | | A1047 | 28.705 | 31.565 | 7.004 | 1.00 46.85 | N |
| ATOM | 351 | | | A1047 | 28.318 | 33.042 | 5.289 | 1.00 46.67 | N |
| ATOM | 352 | С | | A1047 | 23.800 | 38:082 | 7.074 | 1.00 39.44 | С |
| ATOM | 353 | Ö | | A1047 | 23.397 | 38.100 | 8.236 | 1.00 38.89 | 0 |
| ATOM | 354 | N | | A1048 | 23.914 | 39.178 | 6.338 | 1.00 37.81 | N |
| ATOM | 355 | CA | | A1048 | 23.550 | 40.475 | 6.871 | 1.00 36.41 | C |
| ATOM | 356 | СВ | | A1048 | 24.011 | 41.576 | 5.920 | 1.00 36.74 | Ċ |
| ATOM | 357 | CG | | A1048 | 24.106 | 42.940 | 6.565 | 1.00 37.57 | c |
| MOTA | 358 | CD | | A1048 | 24.476 | 44.024 | 5.578 | 1.00 38.09 | Č |
| MOTA | 359 | | | A1048 | 24.860 | 45.132 | 5.965 | 1.00 38.67 | Õ |
| ATOM | 360 | | | A1048 | 24.351 | 43.717 | 4.295 | 1.00 38.03 | N |
| ATOM | 361 | C | | A1048 | 22.037 | 40.561 | 7.074 | 1.00 35.21 | C |
| | ~ ~ ~ | _ | | | , | | | | _ |

| ATOM | 362 | 0 | GLN | A1048 | 21.567 | 41.201 | 8.015 | 1.00 34.68 | 0 |
|------|-----|-----|-----|-------|--------|--------|--------|------------|-----|
| ATOM | 363 | N | ILE | A1049 | 21.279 | 39.919 | 6.189 | 1.00 33.75 | N |
| ATOM | 364 | CA | ILE | A1049 | 19.826 | 39.934 | 6.295 | 1.00 32.76 | С |
| ATOM | 365 | CB | ILE | A1049 | 19.146 | 39.436 | 4.987 | 1.00 32.88 | С |
| ATOM | 366 | | | A1049 | 17.628 | 39.437 | 5.153 | 1.00 32.63 | C |
| ATOM | 367 | | | A1049 | 19.536 | 40.333 | 3.808 | 1.00 32.63 | č |
| ATOM | 368 | | | A1049 | 19.070 | 41.776 | 3.930 | 1.00 32.59 | c |
| | | | | | | | | | |
| ATOM | 369 | C | | A1049 | 19.366 | 39.062 | 7.466 | 1.00 31.99 | C |
| MOTA | 370 | 0 | | A1049 | 18.480 | 39.456 | 8.223 | 1.00 31.76 | 0 |
| ATOM | 371 | N | | A1050 | 19.964 | 37.883 | 7.611 | 1.00 31.37 | N |
| ATOM | 372 | CA | GLU | A1050 | 19.610 | 36.982 | 8.707 | 1.00 31.34 | С |
| ATOM | 373 | CB | GLU | A1050 | 20.362 | 35.648 | 8.591 | 1.00 32.61 | С |
| ATOM | 374 | CG | GLU | A1050 | 20.706 | 34.980 | 9.944 | 1.00 36.11 | C |
| ATOM | 375 | CD | GLU | A1050 | 19.482 | 34.642 | 10.819 | 1.00 37.78 | C |
| ATOM | 376 | OE1 | GLU | A1050 | 19.674 | 34.340 | 12.024 | 1.00 39.05 | 0 |
| ATOM | 377 | | | A1050 | 18.339 | 34.671 | 10.311 | 1.00 38.44 | . 0 |
| ATOM | 378 | C | | A1050 | 19.929 | 37.642 | 10.047 | 1.00 30.27 | C |
| ATOM | 379 | 0 | | A1050 | 19.172 | 37.494 | 11.014 | 1.00 30.09 | Ō |
| ATOM | 380 | N | | A1051 | 21.041 | 38.372 | 10.107 | 1.00 28.49 | N |
| | | | | | | | | 1.00 23.43 | |
| ATOM | 381 | CA | | A1051 | 21.398 | 39.040 | 11.343 | | С |
| MOTA | 382 | CB | | A1051 | 22.747 | 39.750 | 11.244 | 1.00 26.82 | С |
| ATOM | 383 | CG | | A1051 | 23.032 | 40.565 | 12.484 | 1.00 26.72 | С |
| ATOM | 384 | CD1 | TYR | A1051 | 22.657 | 41.906 | 12.569 | 1.00 26.89 | C |
| ATOM | 385 | CE1 | TYR | A1051 | 22.830 | 42.627 | 13.750 | 1.00 26.37 | C |
| ATOM | 386 | CD2 | TYR | A1051 | 23.590 | 39.970 | 13.612 | 1.00 26.66 | C |
| ATOM | 387 | CE2 | TYR | A1051 | 23.761 | 40.676 | 14.786 | 1.00 26.28 | С |
| ATOM | 388 | CZ | | A1051 | 23.381 | 42.000 | 14.852 | 1.00 26.29 | С |
| ATOM | 389 | ОН | | A1051 | 23.554 | 42.688 | 16.031 | 1.00 26.92 | 0 |
| ATOM | 390 | С | | A1051 | 20.332 | 40.069 | 11.670 | 1.00 26.31 | С |
| ATOM | 391 | ō | | A1051 | 19.893 | 40.189 | 12.811 | 1.00 25.81 | Ō |
| ATOM | 392 | N | | A1052 | 19.927 | 40.812 | 10.650 | 1.00 25.22 | Ŋ |
| ATOM | 393 | | | A1052 | 18.923 | 41.845 | 10.809 | 1.00 24.40 | C |
| | | CA | | | | | 9.532 | | C |
| ATOM | 394 | CB | | A1052 | 18.854 | 42.685 | | 1.00 24.44 | |
| ATOM | 395 | CG | | A1052 | 17.719 | 43.703 | 9.465 | 1.00 25.24 | С |
| ATOM | 396 | | | A1052 | 17.904 | 44.780 | 10.533 | 1.00 24.85 | C |
| ATOM | 397 | | | A1052 | 17.692 | 44.314 | 8.081 | 1.00 25.55 | C |
| MOTA | 398 | С | | A1052 | 17.551 | 41.242 | 11.126 | 1.00 23.78 | C |
| ATOM | 399 | 0 | LEU | A1052 | 16.808 | 41.771 | 11.957 | 1.00 23.28 | 0 |
| ATOM | 400 | N | ALA | A1053 | 17.227 | 40.134 | 10.459 | 1.00 22.87 | N |
| ATOM | 401 | CA | ALA | A1053 | 15.948 | 39.459 | 10.655 | 1.00 22.13 | C |
| ATOM | 402 | CB | ALA | A1053 | 15.780 | 38.354 | 9.619 | 1.00 21.79 | C |
| ATOM | 403 | С | ALA | A1053 | 15.858 | 38.875 | 12.066 | 1.00 21.81 | С |
| ATOM | 404 | 0 | | A1053 | 14.841 | 39.022 | 12.748 | 1.00 21.24 | 0 |
| ATOM | 405 | N | | A1054 | 16.932 | 38.215 | 12.497 | 1.00 21.35 | N |
| ATOM | 406 | CA | | A1054 | 16.953 | 37.624 | 13.819 | 1.00 20.95 | С |
| ATOM | 407 | C | | A1054 | 16.707 | 38.649 | 14.910 | 1.00 20.80 | Ċ |
| ATOM | 408 | Ö | | A1054 | 15.890 | 38.428 | 15.803 | 1.00 20.64 | 0 |
| ATOM | 409 | Ŋ | | A1055 | 17.419 | 39:769 | 14.845 | 1.00 20.73 | N |
| ATOM | 410 | CA | | A1055 | 17.255 | 40.822 | 15.843 | 1.00 21.15 | C |
| | | | | | | | | | |
| ATOM | 411 | CB | | A1055 | 18.254 | 41.959 | 15.586 | 1.00 20.76 | C |
| ATOM | 412 | CG | | A1055 | 19.514 | 41.893 | 16.444 | 1.00 20.45 | |
| ATOM | 413 | CD | | A1055 | 20.238 | 40.562 | 16.281 | 1.00 20.93 | C |
| ATOM | 414 | NE | | A1055 | 21.323 | 40.413 | 17.249 | 1.00 20.92 | N |
| MOTA | 415 | CZ | | A1055 | 22.109 | 39.344 | 17.337 | 1.00 21.08 | C |
| ATOM | 416 | | | A1055 | 21.937 | 38.314 | 16.515 | 1.00 21.54 | N |
| MOTA | 417 | NH2 | ARG | A1055 | 23.073 | 39.308 | 18.246 | 1.00 20.48 | N |
| ATOM | 418 | С | ARG | A1055 | 15.822 | 41.355 | 15.834 | 1.00 20.82 | С |
| | | | | | | | | | |

| ATOM | 419 | 0 | ARG | A1055 | 15.235 | 41.597 | 16.884 | 1.00 19.96 | 0 |
|--------------|------------|----------|-------|----------------|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 420 | N | TRP | A1056 | 15.272 | 41.535 | 14.638 | 1.00 21.33 | N |
| MOTA | 421 | CA | TRP | A1056 | 13.907 | 42.018 | 14.481 | 1.00 21.83 | С |
| ATOM | 422 | CB | TRP | A1056 | 13.597 | 42.252 | 12.995 | 1.00 23.26 | С |
| MOTA | 423 | CG | TRP | A1056 | 12.117 | 42.342 | 12.688 | 1.00 25.60 | С |
| MOTA | 424 | CD2 | TRP | A1056 | 11.384 | 43.518 | 12.326 | 1.00 26.69 | С |
| MOTA | 425 | CE2 | TRP | A1056 | 10.026 | 43.140 | 12.186 | 1.00 27.05 | С |
| ATOM | 426 | CE3 | TRP | A1056 | 11.741 | 44.852 | 12.106 | 1.00 27.71 | С |
| ATOM | 427 | CD1 | TRP | A1056 | 11.199 | 41.324 | 12.745 | 1.00 26.25 | С |
| ATOM | 428 | NE1 | TRP | A1056 | 9.942 | 41.798 | 12.448 | 1.00 27.38 | N |
| MOTA | 429 | CZ2 | TRP | A1056 | 9.025 | 44.048 | 11.839 | 1.00 28.05 | С |
| ATOM | 430 | CZ3 | TRP | A1056 | 10.741 | 45.763 | 11.757 | 1.00 29.41 | С |
| MOTA | 431 | | | A1056 | 9.397 | 45.353 | 11.628 | 1.00 28.81 | C |
| ATOM | 432 | С | | A1056 | 12.956 | 40.973 | 15.059 | 1.00 21.40 | C |
| ATOM | 433 | 0 | | A1056 | 11.999 | 41.299 | 15.754 | 1.00 21.32 | 0 |
| ATOM | 434 | N | | A1057 | 13.233 | 39.714 | 14.752 | 1.00 20.70 | N |
| ATOM | 435 | CA . | | A1057 | 12.429 | 38.605 | 15.231 | 1.00 20.76 | C |
| ATOM | 436 | CB | | A1057 | 12.956 | 37.293 | 14.632 | 1.00 21.29 | C |
| ATOM | 437 | OG | | A1057 | 12.032 | 36.234 | 14.815 | 1.00 23.54 | 0 |
| ATOM | 438 | С | | A1057 | 12.498 | 38.559 | 16.760 | 1.00 20.11 | C |
| ATOM | 439 | 0 | | A1057 | 11.484 | 38.361 | 17.438 | 1.00 19.93 | 0 |
| ATOM | 440 | N | | A1058 | 13.698 | 38.750 | 17.303 | 1.00 19.35 | N |
| MOTA | 441 | CA | | A1058 | 13.881 | 38.727 | 18.751 | 1.00 18.89 | C |
| ATOM | 442 | CB | | A1058 | 15.373 | 38.780 | 19.098 | 1.00 18.02 1.00 18.51 | C C |
| ATOM | 443 | C | | A1058 | 13.139 | 39.865 | 19.448 | | Ö |
| ATOM | 444 | 0 | | A1058 | 12.502 | 39.657 | 20.482 | 1.00 17.31 | |
| ATOM | 445 | N | | A1059 | 13.213 | 41.062 | 18.875 | 1.00 19.01 | N C |
| ATOM | 446 | CA | | A1059 | .12.560 | 42.230 | 19.470 | 1.00 20.07 | C |
| ATOM | 447 | CB | | A1059 | 13.026 14.539 | 43.513 43.671 | 18.771 18.811 | 1.00 19.92 1.00 20.81 | C |
| ATOM | 448 | CG | | A1059 A1059 | 15.003 | 45.101 | 18.534 | 1.00 20.31 | Č |
| ATOM | 449 450 | CD CE | | A1059 | 16.530 | 45.190 | 18.538 | 1.00 21.30 | Č |
| ATOM ATOM | 451 | NZ | | A1059 | 17.028 | 46.597 | 18.453 | 1.00 21.30 | N |
| ATOM | 452 | C | | A1059 | 11.045 | 42.112 | 19.420 | 1.00 20.60 | C |
| ATOM | 453 | 0 | | A1059 | 10.341 | 42.601 | 20.309 | 1.00 19.75 | Ō |
| ATOM | 454 | N | | A1060 | 10.550 | 41.448 | 18.381 | 1.00 21.44 | N |
| ATOM | 455 | CA | | A1060 | 9.118 | 41.246 | 18.234 | 1.00 22.69 | C |
| ATOM | 456 | CB | | A1060 | 8.783 | 40.742 | 16.832 | 1.00 24.22 | С |
| ATOM | 457 | CG | | A1060 | 7.303 | 40.761 | 16.521 | 1.00 27.42 | C |
| MOTA | 458 | CD | | A1060 | 6.730 | 42.169 | 16.542 | 1.00 29.59 | С |
| MOTA | 459 | OE1 | GLU | A1060 | 7.314 | 43.053 | 15.866 | 1.00 29.73 | 0 |
| MOTA | 460 | OE2 | GLU | A1060 | 5.700 | 42.386 | 17.229 | 1.00 30.63 | 0 |
| ATOM | 461 | С | GLU | A1060 | 8.651 | 40.220 | 19.263 | 1.00 22.63 | C |
| MOTA | 462 | 0 | GLU | A1060 | 7.631 | 40.418 | 19.932 | 1.00 22.87 | 0 |
| MOTA | 463 | N | ALA | A1061 | 9.395 | 39.125 | 19.391 | 1.00 22.05 | N |
| MOTA | 464 | CA | ALA | A1061 | 9.012 | 38.091 | 20.346 | 1.00 22.06 | С |
| MOTA | 465 | CB | ALA | A1061 | 9.967 | 36.899 | 20.266 | 1.00 21.94 | С |
| MOTA | 466 | С | ALA | A1061 | 8.997 | 38:663 | 21.755 | 1.00 22.04 | С |
| MOTA | 467 | 0 | | A1061 | 8.106 | 38.359 | 22.539 | 1.00 21.13 | 0 |
| ATOM | 468 | N | | A1062 | 9.978 | 39.506 | 22.063 | 1.00 22.38 | N |
| MOTA | 469 | CA | | A1062 | 10.055 | 40.119 | 23.380 | 1.00 23.29 | C |
| ATOM | 470 | CB | | A1062 | 11.348 | 40.918 | 23.532 | 1.00 22.75 | C |
| ATOM | 471 | CG | | A1062 | 11.440 | 41.648 | 24.833 | 1.00 22.71 | C |
| ATOM | 472 | | | A1062 | 10.804 | 42.876 | 25.003 | 1.00 22.28 | C |
| MOTA | 473 | | | A1062 | 12.107 | 41.080 | 25.914 | 1.00 22.60 | C |
| ATOM | 474 | | | : A1062 | 10.828 | 43.529 | 26.232 | 1.00 22.88 | c c |
| ATOM | 475 | CE2 | . PHF | A1062 | 12.138 | 41.722 | 27.154 | 1.00 22.54 | C |

| ATOM | 476 | CZ | PHE | A1062 | 11.497 | 42.951 | 27.314 | 1.00 22.78 | С |
|------|-----|-----|-----|-------|--------|--------|---------|------------|---|
| ATOM | 477 | С | PHE | A1062 | 8.865 | 41.030 | 23.667 | 1.00 24.27 | C |
| ATOM | 478 | 0 | PHE | A1062 | 8.302 | 41.002 | 24.765 | 1.00 24.37 | 0 |
| ATOM | 479 | N | SER | A1063 | 8.498 | 41.843 | 22.681 | 1.00 25.39 | N |
| ATOM | 480 | CA | SER | A1063 | 7.373 | 42.751 | 22.818 | 1.00 26.79 | C |
| ATOM | 481 | CB | SER | A1063 | 7.196 | 43.580 | 21.542 | 1.00 27.55 | С |
| ATOM | 482 | OG | SER | A1063 | 8.184 | 44.598 | 21.464 | 1.00 28.80 | 0 |
| MOTA | 483 | С | | A1063 | 6.108 | 41.965 | 23.094 | 1.00 27.26 | С |
| ATOM | 484 | 0 | | A1063 | 5.271 | 42.366 | 23.897 | 1.00 27.47 | 0 |
| ATOM | 485 | N | | A1064 | 5.963 | 40.840 | 22.421 | 1.00 28.03 | N |
| ATOM | 486 | CA | | A1064 | 4.793 | 40.018 | 22.637 | 1.00 29.08 | С |
| ATOM | 487 | CB | | A1064 | 4.725 | 38.936 | 21.566 | 1.00 28.90 | С |
| ATOM | 488 | CG | | A1064 | 4.426 | 39.521 | 20:195 | 1.00 30.31 | С |
| ATOM | 489 | CD | | A1064 | 4.605 | 38.519 | 19.075 | 1.00 31.26 | С |
| ATOM | 490 | CE | | A1064 | 3.733 | 37.309 | 19.269, | 1.00 32.24 | Ć |
| ATOM | 491 | NZ | | A1064 | 3.887 | 36.361 | 18.141 | 1.00 33.56 | N |
| ATOM | 492 | C | | A1064 | 4.866 | 39.428 | 24.043 | 1.00 29.71 | С |
| ATOM | 493 | Ö | | A1064 | 3.886 | 39.467 | 24.788 | 1.00 29.61 | 0 |
| ATOM | 494 | N | | A1065 | 6.043 | 38.926 | 24.413 | 1.00 30.48 | N |
| ATOM | 495 | CA | | A1065 | 6.263 | 38.341 | 25.732 | 1.00 31.56 | С |
| ATOM | 496 | CB | | A1065 | 7.739 | 38.022 | 25.917 | 1.00 31.00 | C |
| ATOM | 497 | C | | A1065 | 5.780 | 39.269 | 26.851 | 1.00 32.65 | С |
| ATOM | 498 | 0 | | A1065 | 5.300 | 38.807 | 27.882 | 1.00 31.64 | 0 |
| ATOM | 499 | N | | A1066 | 5.922 | 40.574 | 26.646 | 1.00 34.63 | N |
| ATOM | 500 | CA | | A1066 | 5.479 | 41.557 | 27.630 | 1.00 37.05 | C |
| ATOM | 501 | CB | | A1066 | 6.245 | 42.874 | 27.458 | 1.00 37.61 | C |
| ATOM | 502 | CG | | A1066 | 7.710 | 42.808 | 27.867 | 1.00 39.52 | C |
| ATOM | 503 | SD | | A1066 | 8.007 | 43.039 | 29.649 | 1.00 41.34 | S |
| ATOM | 504 | CE | | A1066 | 8.983 | 44.550 | 29.647 | 1.00 40.03 | c |
| ATOM | 505 | C | | A1066 | 3.985 | 41.798 | 27.435 | 1.00 38.24 | Č |
| MOTA | 506 | .0 | | A1066 | 3.313 | 42.364 | 28.295 | 1.00 38.31 | Ö |
| ATOM | 507 | N | | A1067 | 3.473 | 41.353 | 26.293 | 1.00 39.97 | N |
| ATOM | 508 | CA | | A1067 | 2.065 | 41.524 | 25.996 | 1.00 42.23 | C |
| ATOM | 509 | C | | A1067 | 1.716 | 42.953 | 25.623 | 1.00 43.61 | Ċ |
| ATOM | 510 | Ö | | A1067 | 1.055 | 43.658 | 26.383 | 1.00 44.09 | 0 |
| ATOM | 511 | N | | A1068 | 2.167 | 43.387 | 24.452 | 1.00 44.84 | N |
| MOTA | 512 | CA | | A1068 | 1.889 | 44.739 | 23.985 | 1.00 46.14 | С |
| ATOM | 513 | CB | | A1068 | 3.165 | 45.419 | 23.444 | 1.00 45.80 | С |
| ATOM | 514 | OG1 | 1 | A1068 | 3.639 | 44.703 | 22.297 | 1.00 45.63 | 0 |
| ATOM | 515 | | | A1068 | 4.249 | 45.434 | 24.500 | 1.00 45.44 | С |
| ATOM | 516 | C | | A1068 | 0.854 | 44.654 | 22.868 | 1.00 47.39 | С |
| ATOM | 517 | Ō | | A1068 | 0.473 | 45.661 | 22.270 | 1.00 47.66 | 0 |
| ATOM | 518 | N | | A1069 | 0.409 | 43.432 | 22.592 | 1.00 48.83 | N |
| ATOM | 519 | CA | | A1069 | -0.585 | 43.211 | 21.555 | 1.00 50.40 | C |
| MOTA | 520 | C | | A1069 | -0.073 | | | | C |
| ATOM | 521 | Ö | | A1069 | 0.661 | 42.716 | 19.569 | 1.00 51.45 | 0 |
| ATOM | 522 | N | | A1070 | -0.473 | 44.665 | 19.637 | 1.00 52.38 | N |
| ATOM | 523 | CA | | A1070 | -0.061 | 45:102 | 18.308 | 1.00 53.00 | С |
| ATOM | 524 | CB | | A1070 | -1.285 | 45.483 | 17.444 | 1.00 53.24 | С |
| ATOM | 525 | | | A1070 | -2.148 | 44.245 | 17.194 | 1.00 53.03 | С |
| ATOM | 526 | | | A1070 | -2.102 | 46.575 | 18.145 | 1.00 53.21 | С |
| ATOM | 527 | | | A1070 | -3.310 | 47.043 | 17.350 | 1.00 53.51 | С |
| ATOM | 528 | C | | A1070 | 0.850 | 46.316 | 18.471 | 1.00 53.30 | С |
| ATOM | 529 | Ö | | A1070 | 1.800 | 46.506 | 17.705 | 1.00 53.48 | 0 |
| ATOM | 530 | N | | A1071 | 0.544 | 47.137 | 19.473 | 1.00 53.35 | N |
| ATOM | 531 | CA | | A1071 | 1.344 | 48.321 | 19.771 | 1.00 53.45 | C |
| ATOM | 532 | CB | | A1071 | 0.643 | 49.183 | 20.816 | 1.00 53.58 | С |
| | | | | | | | | | |

| ATOM | 533 | OG | SER | A1071 | 0.57 | 77 48.494 | 22.058 | 1.00 9 | 54.00 | 0 |
|------|-----|----|-----|-------|------|-----------|----------|--------|--------------|--------|
| ATOM | 534 | С | SER | A1071 | 2.63 | 31 47.765 | 20.360 | 1.00 9 | 53.38 | С |
| ATOM | 535 | 0 | SER | A1071 | 2.59 | 96 46.720 | 21.019 | 1.00 9 | 53.61 | 0 |
| MOTA | 536 | N | LYS | A1072 | 3.76 | 63 48.431 | | 1.00 5 | 52.81 | N |
| ATOM | 537 | CA | LYS | A1072 | 5.01 | 19 47.908 | 20.680 | 1.00 9 | 52.05· | С |
| ATOM | 538 | СВ | LYS | A1072 | 5.85 | | | 1.00 9 | 52.53 | С |
| ATOM | 539 | CG | LYS | A1072 | 5.06 | | | 1.00 9 | | С |
| ATOM | 540 | ÇD | | A1072 | 4.0 | | | 1.00 | | Ċ |
| ATOM | 541 | CE | | A1072 | 4.75 | | | 1.00 9 | | C |
| ATOM | 542 | NZ | | A1072 | 3.72 | | | 1.00 | | N |
| ATOM | 543 | C | | A1072 | 5.89 | | | 1.00 | | C |
| ATOM | 544 | Ō | | A1072 | 5.58 | | | 1.00 | | 0 |
| ATOM | 545 | N | | A1073 | 7.00 | | | 1.00 | | N |
| ATOM | 546 | CA | | A1073 | 7.98 | | | 1.00 | | C |
| ATOM | 547 | CB | | A1073 | 8.78 | | | 1.00 | | č |
| ATOM | 548 | CG | | A1073 | 8.1 | | | 1.00 | | Č |
| ATOM | 549 | | | A1073 | 6.8 | | | 1.00 | | Č |
| ATOM | 550 | | | A1073 | 9.0 | | | 1.00 | | Č |
| ATOM | 551 | C | | A1073 | 8.9 | | | 1.00 | | Č |
| ATOM | 552 | Ö | | A1073 | 8.9 | | | 1.00 | | . 0 |
| ATOM | 553 | Ŋ | | A1074 | 9.7 | | | 1.00 | | N |
| ATOM | 554 | CA | | A1074 | 10.6 | | | 1.00 | | C |
| ATOM | 555 | C | | A1074 | 11.7 | | | 1.00 | | Č |
| ATOM | 556 | 0 | | A1074 | 12.3 | | | 1.00 | | 0 |
| ATOM | 557 | N | | A1075 | 11.9 | | | 1.00 | | N |
| ATOM | 558 | CA | | A1075 | 12.9 | | | 1.00 | | c c |
| ATOM | 559 | CB | | A1075 | 12.8 | | | 1.00 | | č |
| ATOM | 560 | CG | | A1075 | 11.9 | | | 1.00 | | č |
| ATOM | 561 | | | A1075 | 10.9 | | | 1.00 | | c |
| MOTA | 562 | | | A1075 | 12.1 | | | 1.00 | | C |
| MOTA | 563 | | | A1075 | 10.0 | | | 1.00 | | C |
| ATOM | 564 | | | A1075 | 11.2 | | | 1.00 | | c |
| ATOM | 565 | CZ | | A1075 | 10.2 | | | 1.00 | | Č |
| ATOM | 566 | C | | A1075 | 14.3 | | | 1.00 | | c |
| ATOM | 567 | 0 | | A1075 | 15.2 | | | 1.00 | | ő |
| ATOM | 568 | N | | A1076 | 14.5 | | | 1.00 | | N |
| ATOM | 569 | CA | | A1076 | 15.7 | | | | 35.77 | C |
| ATOM | 570 | CB | | A1076 | 15.8 | | | | 35.98 | C |
| ATOM | 571 | CG | | A1076 | 16.0 | | | 1.00 | | C |
| ATOM | 572 | CD | | A1076 | 17.3 | | | | 35.92 | Č |
| ATOM | 573 | | | A1076 | 18.4 | | | | 36.68 | Õ |
| ATOM | 574 | | | A1076 | 17.1 | | | | 35.79 | N |
| ATOM | 575 | C | | A1076 | 15.9 | | | | 34.84 | C |
| ATOM | 576 | Ö | | A1076 | 17.0 | | | | 34.87 | ō |
| ATOM | 577 | N | | A1077 | 14.8 | | 3 22.202 | | | N |
| ATOM | 578 | CA | | A1077 | 14.8 | | | | 32.88 | C |
| ATOM | 579 | CB | | A1077 | 13.4 | | | | 34.04 | C |
| ATOM | 580 | CG | | A1077 | 13.1 | | | | 35.48 | С |
| ATOM | 581 | | | A1077 | 13.8 | | | | 36.31 | o |
| ATOM | 582 | | | A1077 | 12.2 | | | | 36.39 | 0 |
| ATOM | 583 | C | | A1077 | 15.1 | | | | 31.37 | С |
| ATOM | 584 | Ö | | A1077 | 15.2 | | | | 30.93 | Ō |
| ATOM | 585 | N | | A1078 | 15.4 | | | | 29.66 | N |
| ATOM | 586 | CA | | A1078 | 15.7 | | | | 28.12 | С |
| ATOM | 587 | CB | | A1078 | 14.6 | | | | 28.40 | C |
| ATOM | 588 | CG | | A1078 | 13.2 | | | | 28.65 | С |
| ATOM | 589 | | | A1078 | 12.1 | | | | 28.42 | C |
| | | · | | | | | | • | - | _ |

| ATOM | 590 | CD2 | LEU | A1078 | | 13.232 | 45.784 | 24.485 | | 28.42 | С |
|--------------|------------|-----------|-----|----------------|---|------------------|------------------|------------------|------|-------|---|
| ATOM | 591 | С | | A1078 | | 17.029 | 46.469 | 22.317 | 1.00 | 26.77 | С |
| ATOM | 592 | 0 | LEU | A1078 | | 17.256 | 46.963 | 21.219 | 1.00 | 26.91 | 0 |
| ATOM | 593 | N | GLU | A1079 | | 17.892 | 45.683 | 22.944 | 1.00 | 25.48 | N |
| ATOM | 594 | CA | GLU | A1079 | | 19.166 | 45.352 | 22.330 | 1.00 | 24.50 | С |
| ATOM | 595 | CB | GLU | A1079 | ; | 20.287 | 46.202 | 22.921 | 1.00 | 24.22 | С |
| ATOM | 596 | CG | GLU | A1079 | | 21.561 | 46.128 | 22.114 | 1.00 | 23.64 | C |
| ATOM | 597 | CD | GLU | A1079 | | 22.638 | 47.051 | 22.635 | 1.00 | 24.07 | С |
| ATOM | 598 | OE1 | GLU | A1079 | | 23.079 | 46.862 | 23.791 | 1.00 | 23.41 | 0 |
| ATOM | 599 | OE2 | GLU | A1079 | | 23.044 | 47.967 | 21.883 | 1.00 | 24.29 | 0 |
| ATOM | 600 | C T | GLU | A1079 | | 19.512 | 43.885 | 22.488 | 1.00 | 23.86 | С |
| ATOM | 601 | 0 | GLU | A1079 | | 19.341 | 43.305 | 23.560 | 1.00 | 23.77 | 0 |
| ATOM | 602 | N | | A1080 | | 20.003 | 43.291 | 21.408 | 1.00 | 23.09 | N |
| ATOM | 603 | CA | VAL | A1080 | | 20.377 | 41.888 | 21.411 | 1.00 | 22.78 | С |
| ATOM | 604 | CB | | A1080 | | 19.413 | 41.032 | 20.529 | 1.00 | 22.41 | С |
| ATOM | 605 | | | A1080 | | 20.005 | 39.649 | 20.284 | | 21.10 | С |
| ATOM | 606 | | | A1080 | | 18.059 | 40.893 | 21.224 | | 21.12 | С |
| ATOM | 607 | C | | A1080 | | 21.800 | 41.707 | 20.909 | | 23.31 | С |
| ATOM | 608 | Õ | | A1080 | | 22.102 | 41.942 | 19.737 | | 23.36 | 0 |
| ATOM | 609 | N | | A1081 | | 22.673 | 41.292 | 21.818 | | 23.52 | N |
| ATOM | 610 | CA | | A1081 | | 24.066 | 41.056 | 21.488 | | 23.32 | C |
| ATOM | 611 | CB | | A1081 | | 24.968 | 41.910 | 22.391 | | 22.81 | Č |
| ATOM | 612 | CG | | A1081 | | 24.725 | 43.426 | 22.313 | | 22.95 | Č |
| ATOM | 613 | | | A1081 | | 25.680 | 44.170 | 23.239 | | 22.31 | Č |
| ATOM | 614 | | | A1081 | | 24.919 | 43.902 | 20.874 | | 23.08 | č |
| ATOM | 615 | C | | A1081 | | 24.347 | 39.576 | 21.709 | | 23.58 | Č |
| MOTA | 616 | 0 | | A1081 | | 23.436 | 38.786 | 21.981 | | 22.36 | ō |
| | 617 | | | A1082 | | 25.430 | 39.204 | 21.582 | | 24.47 | N |
| ATOM | | N | | | | 26.018 | 37.826 | 21.802 | | 25.10 | C |
| ATOM | 618 619 | CA CB | | A1082 A1082 | | 26.745 | 37.301 | 20.564 | | 25.30 | C |
| ATOM | 620 | CG | | A1082 | | 25.798 | 37.072 | 19.406 | | 25.42 | c |
| ATOM | | | | | | | 36.277 | 19.514 | | 26.33 | 0 |
| ATOM | 621 622 | | | A1082 A1082 | | 24.863 26.023 | 37.769 | 18.299 | | 25.02 | N |
| ATOM | | | | | | | 37.774 | 23.042 | | 25.09 | C |
| ATOM | 623 | С | | A1082 | | 26.897 27.802 | 38.586 | 23.197 | | 24.45 | 0 |
| ATOM | 624 | 0 | | A1082 | | 26.614 | 36.825 | 23.137 | | 26.16 | N |
| ATOM | 625 | N | | A1083 | | | | 25.180 | | 26.89 | C |
| ATOM | 626 | CA | | E801A | | 27.365 | 36.697 36.048 | 26.264 | | 26.14 | C |
| ATOM | 627 | CB | | A1083 | | 26.484 | 34.600 | 25.952 | | 25.65 | c |
| ATOM ATOM | 628 629 | CG OD1 | | A1083 A1083 | | 26.094 25.289 | 34.006 | 26.668 | | 25.06 | 0 |
| ATOM | | | | A1083 | | 26.665 | 34.000 | 24.900 | | 25.04 | N |
| | 630 631 | C | | A1083 | | 28.691 | 35.953 | 25.044 | | 27.81 | C |
| ATOM | 632 | 0 | | A1083 | | 29.098 | 35.595 | 23.939 | | 27.57 | 0 |
| MOTA | 633 | N | | A1083 | | 29.373 | 35.729 | 26.162 | | 29.55 | N |
| MOTA | | | | | | 30.656 | | | | 31.72 | Ċ |
| ATOM | 634 | CA | | A1084 | | 31.382 | 35.041 | 27.465 | | 32.66 | d |
| ATOM ATOM | 635 636 | CB CG | | A1084 A1084 | | 30.618 | 34.574 | 28.685 | | 34.91 | Ċ |
| | 637 | CD | | A1084 | | 31.407 | 34:752 | 29.998 | | 36.48 | ď |
| ATOM | | | | A1084 | | 32.421 | 34.752 | 30.192 | | 37.32 | Ö |
| ATOM | 638 639 | | | A1084 | | 31.022 | 35.601 | 30.192 | | 37.46 | d |
| MOTA | | | | A1084 | | 30.532 | 33.603 | 25.584 | | 32.13 | C |
| ATOM | 640 | С | | | | | | | | 32.13 | C |
| ATOM | 641 | 0 | | A1084 | | 31.522 | 33.007 | 25.186 | | | N |
| ATOM | 642 | N CA | | A1085 | | 29.322 | 33.052 | 25.578 | | 32.33 | C |
| ATOM | 643 | CA | | A1085 | | 29.118 | 31.703 30.950 | 25.061 25.866 | | 34.65 | C |
| ATOM | 644 | CB | | A1085 | | 28.057 | 30.506 | 27.238 | | 37.26 | Ċ |
| ATOM | 645 | CG | | | | 28.525 29.588 | 29.432 | 27.230 | | 39.70 | |
| ATOM | 646 | CD | AKG | A1085 | | 23.350 | 67.436 | 21.112 | 1.00 | 27.10 | |

| MOTA | 647 | NE | ARG | A1085 | 30.430 | 29.337 | 28.303 | 1.00 42.39 | N | i |
|--------------|------------|----------|-----|----------------|------------------|------------------|------------------|------------|-----|---|
| ATOM | 648 | CZ | ARG | A1085 | 31.329 | 28.375 | 28.501 | 1.00 43.44 | С | , |
| MOTA | 649 | NH1 | ARG | A1085 | 32.062 | 28.363 | 29.611 | 1.00 44.05 | N | i |
| ATOM | 650 | NH2 | ARG | A1085 | 31.482 | 27.415 | 27.593 | 1.00 43.73 | N | i |
| ATOM | 651 | С | ARG | A1085 | 28.682 | 31.788 | 23.606 | 1.00 31.86 | C | : |
| MOTA | 652 | 0 | ARG | A1085 | 28.369 | 30.775 | 22.983 | 1.00 32.12 | 0 |) |
| MOTA | 653 | N | GLY | A1086 | 28.664 | 33.006 | 23.070 | 1.00 30.59 | N | l |
| MOTA | 654 | CA | GLY | A1086 | 28.275 | 33.206 | 21.687 | 1.00 29.15 | Ò | : |
| ATOM | 655 | С | GLY | A1086. | 26.779 | 33.208 | 21.427 | 1.00 28.22 | C | : |
| ATOM | 656 | 0 | GLY | A1086 | 26.347 | 33.336 | 20.287 | 1.00 28.76 | C |) |
| ATOM | 657 | N | ALA | A1087 | 25.980 | 33.079 | 22.476 | 1.00 26.78 | N | |
| ATOM | 658 | CA | ALA | A1087 | 24.536 | 33.052 | 22.313 | 1.00 25.40 | C | |
| ATOM | 659 | CB | ALA | A1087 | 23.907 | 32.162 | 23.378 | 1.00 24.76 | C | |
| ATOM | 660 | С | ALA | A1087 | 23.936 | 34.448 | 22.390 | 1.00 24.84 | C | |
| MOTA | 661 | 0 | ALA | A1087 | 24.417 | 35.304 | 23.142 | 1.00 24.29 | C | |
| MOTA | 662 | N | PRO | A1088 | 22.886 | 34.703 | 21.591 | 1.00 23.94 | N | |
| MOTA | 663 | CD | PRO | A1088 | 22.363 | 33.864 | 20.496 | 1.00 23.58 | C | |
| MOTA | 664 | CA | PRO | A1088 | 22.234 | 36.009 | 21.601 | 1.00 23.19 | C | |
| MOTA | 665 | CB | PRO | A1088 | 21.303 | 35.944 | 20.388 | 1.00 23.32 | C | |
| ATOM | 666 | CG | | A1088 | 21.019 | 34.482 | 20.239 | 1.00 23.28 | C | |
| MOTA | 667 | С | PRO | A1088 | 21.483 | 36.232 | 22.911 | 1.00 22.65 | C | |
| ATOM | 668 | 0 | | A1088 | 20.908 | 35.304 | 23.475 | 1.00 22.59 | | |
| MOTA | 669 | N | | A1089 | 21.518 | 37.464 | 23.407 | 1.00 22.22 | 1 | |
| MOTA | 670 | CA | | A1089 | 20.824 | 37.808 | 24.645 | 1.00 21.73 | C | |
| MOTA | 671 | CB | | A1089 | 21.720 | 37.537 | 25.866 | 1.00 21.31 | | |
| MOTA | 672 | CG | TYR | A1089 | 22.843 | 38.540 | 26.058 | 1.00 20.82 | , (| |
| MOTA | 673 | CD1 | | A1089 | 22.795 | 39.475 | 27.095 | 1.00 20.39 | | 2 |
| MOTA | 674 | CE1 | TYR | A1089 | 23.791 | 40.428 | 27.253 | 1.00 20.46 | | C |
| MOTA | 675 | | | A1089 | 23.931 | 38.582 | 25.177 | 1.00 20.50 | | 2 |
| MOTA | 676 | CE2 | | A1089 | 24.942 | 39.535 | 25.323 | 1.00 20.31 | | 2 |
| MOTA | 677 | CZ | | A1089 | 24.865 | 40.458 | 26.363 | 1.00 21.12 | | 2 |
| MOTA | 678 | OH | | A1089 | 25.844 | 41.421 | 26.507 | 1.00 20.91 | | 0 |
| MOTA | 679 | C | | A1089 | 20.459 | 39.278 | 24.598 | 1.00 21.43 | | 0 |
| ATOM | 680 | 0 | | A1089 | 20.986 | 40.045 | 23.782 | 1.00 21.20 | | 0 |
| ATOM | 681 | N | | A1090 | 19.541 | 39.670 | 25.469 | 1.00 21.81 | | N |
| ATOM | 682 | CA | | A1090 | 19.134 | 41.058 | 25.534 | 1.00 21.85 | | C |
| ATOM | 683 | CB | | A1090 | 17.694 | 41.182 | 26.041 | 1.00 20.99 | | C |
| ATOM | 684 | CG | | A1090 | 16.651 | 40.841 | 25.006 | 1.00 20.79 | | C |
| ATOM | 685 | | | A1090 | 16.294 | 39.519 | 24.755 | 1.00 20.19 | | C |
| ATOM | 686 | | | A1090 | 16.052 | 41.849 | 24.247 | 1.00 20.29 | | C |
| ATOM | 687 | | | A1090 | 15.364 15.122 | 39.207 41.543 | 23.760 23.252 | 1.00 19.79 | | C |
| ATOM | 688 | | | A1090 | 14.778 | 40.221 | 23.232 | 1.00 20.00 | | c |
| ATOM | 689 690 | CZ C | | A1090 | 20.087 | 41.794 | 26.467 | 1.00 19.21 | | C |
| MOTA | 691 | | | A1090 A1090 | 20.087 | 41.460 | 27.643 | 1.00 22.82 | | o |
| ATOM ATOM | 692 | О И | | A1091 | 20.791 | 42.780 | 25.922 | 1.00 22.02 | | N |
| | 693 | | | A1091 | 21.725 | 43.590 | 26.697 | 1.00 24.38 | | C |
| ATOM ATOM | 694 | CA CB | | A1091 | 22.879 | 44:048 | 25.805 | 1.00 24.43 | | C |
| ATOM | 695 | OG | | A1091 | 22.405 | 44.352 | 24.504 | 1.00 25.11 | | o |
| ATOM | 696 | C | | A1091 | 20.979 | 44.805 | 27.248 | | | C |
| MOTA | 697 | 0 | | A1091 | 21.420 | 45.443 | 28.204 | 1.00 24.93 | | 0 |
| ATOM | 698 | И. | | A1091 | 19.854 | 45.124 | 26.618 | 1.00 25.07 | | N |
| ATOM | 699 | CA | | A1092 | 19.023 | 46.235 | 27.046 | 1.00 26.14 | | c |
| ATOM | 700 | CB | | A1092 | 19.357 | 47.517 | 26.258 | 1.00 27.41 | | Ċ |
| ATOM | 701 | CG | | A1092 | 20.779 | 48.089 | 26.463 | 1.00 29.10 | | Ċ |
| ATOM | 702 | CD | | A1092 | 21.096 | 48.475 | 27.918 | 1.00 31.36 | | c |
| ATOM | 703 | | | A1092 | 20.273 | 49.093 | 28.607 | 1.00 32.18 | | o |
| | | | | | | | | | | |

| ATOM | 704 | NE2 | GLN | A1092 | 22.306 | 48.127 | 28.380 | 1.00 31.33 | N |
|--------------|------------|--------|-----|----------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 705 | С | GLN | A1092 | 17.556 | 45.850 | 26.841 | 1.00 25.78 | С |
| ATOM | 706 | 0 | GLN | A1092 | 17.148 | 45.443 | 25.753 | 1.00 25.27 | 0 |
| MOTA | 707 | N | ALA | A1093 | . 16.777 | 45.961 | 27.909 | 1.00 25.60 | N |
| ATOM | 708 | CA | ALA | A1093 | 15.357 | 45.630 | 27.870 | 1.00 25.62 | С |
| ATOM | 709 | CB | ALA | A1093 | 15.171 | 44.110 | 27.867 | 1.00 24.75 | С |
| ATOM | 710 | С | ALA | A1093 | 14.677 | 46.238 | 29.090 | 1.00 25.61 | С |
| MOTA | 711 | 0 | ALA | A1093 | 15.220 | 46.209 | 30.186 | 1.00 25.48 | 0 |
| ATOM | 712 | N | PRO | A1094 | 13.474 | 46.796 | 28.916 | 1.00 26.29 | N |
| MOTA | 713 | CD | | A1094 | 12.668 | 46.878 | 27.682 | 1.00 26.31 | С |
| ATOM | 714 | CA | PRO | A1094 | 12.758 | 47.400 | 30.046 | 1.00 26.85 | С |
| ATOM | 715 | CB | PRO | A1094 | 11.622 | 48.147 | 29.358 | 1.00 26.71 | С |
| ATOM | 716 | CG | | A1094 | 11.292 | 47.223 | 28.222 | 1.00 26.01 | C |
| ATOM | 717 | C | | A1094 | 12.241 | 46.343 | 31.024 | 1.00 27.25 | C |
| MOTA | 718 | 0 | | A1094 | 11.182 | 46.511 | 31.631 | 1.00 28.16 | 0 |
| ATOM | 719 | N | | A1095 | 12.980 | 45.248 | 31.167 | 1.00 26.92 | N |
| ATOM | 720 | CA | | A1095 | 12.571 | 44.181 | 32.069 | 1.00 26.96 | С |
| ATOM | 721 | CB. | | A1095 | 12.234 | 42.918 | 31.279 | 1.00 26.69 | C |
| ATOM | 722 | CG | | A1095 | 11.729 | 41.782 | 32.127 | 1.00 26.67 | C |
| ATOM | 723 | | | A1095 | 12.396 | 40.553 | 32.137 | 1.00 26.30 | C |
| ATOM | 724 | | | A1095 | 10.567 | 41.920 | 32.879 | 1.00 25.87 | C |
| ATOM | 725 | | | A1095 | 11.911 | 39.481 | 32.878 | 1.00 25.90 | |
| ATOM | 726 | | | A1095 | 10.074 | 40.853 | 33.624 | 1.00 25.69 | C |
| ATOM | 727 | CZ | | A1095 | 10.746 | 39.628 | 33.625 | 1.00 26.13 | C |
| ATOM | 728 | С | | A1095 | 13.685 | 43.891 | 33.055 | 1.00 26.99 | |
| ATOM | 729 | 0 | | A1095 | 14.854 | 43.835 | 32.680 | 1.00 27.34 1.00 26.53 | 0 N |
| ATOM | 730 | N | | A1096 | 13.319 | 43.687 | 34.314 35.340 | 1.00 26.73 | C |
| ATOM | 731 | CA | | A1096 | 14.308 | 43.436 | 36.596 | 1.00 27.70 | c |
| ATOM | 732 | CB | | A1096 | 13.973 12.642 | 44.263 44.023 | 37.052 | 1.00 27.70 | 0 |
| ATOM | 733 | OG | | A1096 | 14.500 | 41.968 | 35.715 | 1.00 26.21 | c |
| ATOM | 734 735 | C O | | A1096 A1096 | 15.426 | 41.639 | 36.464 | 1.00 26.51 | 0 |
| ATOM ATOM | 736 | N | | A1090 | 13.420 | 41.033 | 35.198 | 1.00 25.26 | N |
| ATOM | 737 | CA | | A1097 | 13.773 | 39.679 | 35.521 | 1.00 23.20 | c |
| ATOM | 738 | C | | A1097 | 14.633 | 38.918 | 34.529 | 1.00 24.17 | c |
| ATOM | 739 | Ö | | A1097 | 15.383 | 39.512 | 33.758 | 1.00 24.01 | 0 |
| ATOM | 740 | N | | A1098 | 14.526 | 37.594 | 34.552 | 1.00 23.74 | N |
| ATOM | 741 | CA | | A1098 | 15.281 | 36.745 | 33.643 | 1.00 23.42 | C |
| MOTA | 742 | CB | | A1098 | 15.360 | 35.309 | 34.172 | 1.00 24.51 | С |
| MOTA | 743 | CG | | A1098 | 16.177 | 35.141 | 35.444 | 1.00 26.65 | C |
| MOTA | 744 | CD | | A1098 | 16.236 | 33.682 | 35.898 | 1.00 28.23 | С |
| ATOM | 745 | CE | | A1098 | 17.224 | | 37.058 | 1.00 30.02 | С |
| ATOM | 746 | NZ | | A1098 | 17.270 | 32.108 | 37.594 | 1.00 30.95 | N |
| MOTA | 747 | С | LYS | A1098 | 14.602 | 36.730 | 32.287 | 1.00 22.48 | С |
| ATOM | 748 | 0 | LYS | A1098 | 13.374 | 36.671 | 32.192 | 1.00 22.17 | 0 |
| ATOM | 749 | N | | A1099 | 15.419 | 36.782 | 31.241 | 1.00 21.41 | N |
| ATOM | 750 | CA | ILE | A1099 | 14.941 | 36.761 | 29.876 | 1.00 20.15 | C |
| ATOM | 751 | CB | ILE | A1099 | 15.333 | 38:039 | 29.134 | 1.00 19.84 | С |
| MOTA | 752 | CG2 | ILE | A1099 | 14.804 | 37.989 | 27.713 | 1.00.20.13 | С |
| ATOM | 753 | | | A1099 | 14.791 | 39.263 | 29.873 | 1.00 19.76 | С |
| ATOM | 754 | CD1 | ILE | A1099 | 15.218 | 40.583 | 29.262 | 1.00 18.64 | С |
| ATOM | 755 | С | | A1099 | 15.576 | 35.581 | 29.148 | 1.00 19.81 | C |
| ATOM | 756 | 0 | | A1099 | 16.791 | 35.528 | 28.972 | 1.00 20.43 | 0 |
| MOTA | 757 | N | | A1100 | 14.761 | 34.623 | 28.740 | | N |
| MOTA | 758 | CA | | A1100 | 15.277 | 33.480 | 28.005 | | C |
| ATOM | 759 | CB | | A1100 | 14.653 | 32.193 | 28.530 | | C |
| ATOM | 760 | CG | TRE | A1100 | 14.970 | 31.962 | 29.973 | 1.00 17.80 | С |
| | | | | | | | | | |

| ATOM | 761 | CD2 | TRP | A1100 | 16.150 | 31.351 | 30.501 | 1.00 17.39 | | C |
|--------------|--------------|---------|-----|----------------|------------------|------------------|------------------|------------------------|-----|--------|
| MOTA | 762 | | | A1100 | 16.038 | 31.375 | 31.914 | 1.00 17.58 | | C |
| MOTA | 763 | CE3 | TRP | A1100 | 17.294 | 30.787 | 29.921 | 1.00 17.40 | | C |
| MOTA | 764 | | | A1100 | 14.210 | 32.323 | 31.055 | 1.00 17.92 | | C |
| ATOM | 765 | NE1 | TRP | A1100 | 14.844 | 31.972 | 32.222 | 1.00 17.09 | | N |
| ATOM | 766 | CZ2 | TRP | A1100 | 17.030 | 30.851 | 32.759 | 1.00 16.7 | | С |
| ATOM | 767 | CZ3 | TRP | A1100 | 18.283 | 30.268 | 30.763 | 1.00 17.50 | | C |
| ATOM | 768 | CH2 | TRP | A1100 | 18.138 | 30.307 | 32.167 | 1.00 17.0 | | С |
| ATOM | 769 | С | | A1100 | 14.946 | 33.700 | 26.526 | 1.00 17.8 | | С |
| ATOM | 770 | 0 | | A1100 | 13.791 | 33.866 | 26.143 | 1.00 18.0 | | 0 |
| MOTA | 771 | N | | A1101 | 15.987 | 33.725 | 25.707 | 1.00 17.4 | | N |
| MOTA | 772 | CA | LEU | A1101 | 15.852 | 33.967 | 24.290 | 1.00 16.3 | | С |
| ATOM | 773 | CB | | A1101 | 16.469 | 35.325 | 23.955 | 1.00 15.6 | | C |
| ATOM | 774 | CG | | A1101 | 16.715 | 35.601 | 22.468 | 1.00 15.1 | | C |
| ATOM | 775 | | | A1101 | 15.379 | 35.873 | 21.762 | 1.00 13.7 | | C |
| ATOM | 776 | | | A1101 | 17.669 | 36.775 | 22.317 | 1.00 14.2 | | C |
| MOTA | 777 | С | | A1101 | 16.520 | 32.916 | 23.429 | 1.00 16.4 | | C |
| MOTA | 778 | 0 | | A1101 | 17.624 | 32.474 | 23.720 | 1.00 16.3 | | 0 |
| MOTA | 779 | N | | A1102 | 15.847 | 32.520 | 22.356 | 1.00 17.1 | | N C |
| ATOM | 780 | CA | | A1102 | 16.429 | 31.565 | 21.432 | 1.00 17.3 | | C |
| ATOM | 781 | СВ | | A1102 | 15.962 | 30.140 | 21.722 | 1.00 16.6 | | 0 |
| ATOM | 782 | OG | | A1102 | 16.736 | 29.217 | 20.966 | 1.00 15.2 | | C |
| ATOM | 783 | С | | A1102 | 16.052 | 31.965 | 20.011 | 1.00 18.5 | | 0 |
| MOTA | 784 | 0 | | A1102 | 14.902 | 32.319 | 19.727 | 1.00 18.3 1.00 19.2 | | Ŋ |
| ATOM | 785 | | | A1103 | 17.043 | 31.930 | 19.127 | | | C |
| ATOM | 786 | CA | | A1103 | 16.836 | 32.286 | 17.740 | 1.00 20.4 | | C |
| ATOM | 787 | CB | | A1103 | 17.588 | 33.578 | 17.386 | 1.00 20.3 | | C |
| ATOM | 788 | | | A1103 | 17.216 | 34.026 | 15.981 | 1.00 19.8 | | C |
| ATOM | 789 | | | A1103 | 17.240 | 34.675 | 18.399 | 1.00 20.7 | | C |
| ATOM | 790 | | | A1103 | 17.996 | 35.980 | 18.172 16.843 | 1.00 20.0 | | Č |
| ATOM | 791 | C | | A1103 | 17.347 | 31.169 30.551 | 17.121 | 1.00 21.7 | | Õ |
| ATOM | 792 | 0 | | A1103 | 18.373 16.625 | 30.916 | 15.764 | 1.00 21.9 | | N |
| MOTA | 793 | N | | A1104 | 17.015 | 29.884 | 14.823 | 1.00 22.9 | | C |
| ATOM | 794 | CA | | A1104 | 16.334 | 28.556 | 15.185 | 1.00 22.7 | | Č |
| ATOM | 795 | CB | | A1104 | 16.618 | 27.550 | 14.229 | 1.00 21.9 | | ō |
| MOTA | 796 | OG C | | A1104 | 16.607 | 30.322 | 13.421 | 1.00 23.8 | | Ċ |
| MOTA | 797 | С | | A1104 A1104 | 15.698 | 31.139 | 13.246 | 1.00 24.1 | | Ō |
| ATOM | 798 · 799 | O N | | A1104 | 17.283 | 29.787 | 12.417 | 1.00 25.1 | | N |
| ATOM | 800 | CA | | A1105 | 16.943 | 30.144 | 11.049 | 1.00 26.2 | | C |
| ATOM ATOM | 801 | CB | | A1105 | 17.665 | 31.429 | 10.633 | 1.00 26.3 | | С |
| ATOM | 802 | CG | | A1105 | 19.153 | 31.290 | 10.559 | 1.00 27.0 | | С |
| ATOM | 803 | | | A1105 | 19.960 | 30.889 | 9.549 | 1.00 27.0 | | С |
| MOTA | 804 | | | A1105 | 19.980 | 31.551 | 11.630 | 1.00 27.5 | | N |
| ATOM | 805 | | | A1105 | 21.234 | | | 1.00 27.3 | 17 | С |
| ATOM | 806 | | | A1105 | 21.249 | 30.914 | 10.025 | 1.00 27.2 | | N |
| ATOM | 807 | C | | A1105 | 17.276 | | 10.042 | 1.00 26. | 76 | С |
| ATOM | 808 | Ö | | A1105 | 18.031 | | 10.318 | 1.00 26. | 55 | Ο |
| ATOM | 809 | N | | R A1106 | 16.670 | | 8.874 | 1.00 27. | 49 | N |
| ATOM | 810 | CA | | R A1106 | 16.901 | 28.309 | 7.751 | 1.00 28. | 62 | C |
| ATOM | 811 | СВ | | R A1106 | 15.595 | 27.643 | 7.273 | 1.00 28. | 4 4 | С |
| ATOM | 812 | | | R A1106 | 14.721 | | 6.712 | 1.00 27. | | 0 |
| ATOM | 813 | | | R A1106 | 14.901 | 26.954 | 8.447 | 1.00 28. | | С |
| ATOM | 814 | | | R A1106 | 17.381 | 29.299 | 6.698 | 1.00 29. | | С |
| ATOM | 815 | | | R A1106 | 17.685 | 30.442 | | 1.00 29. | | 0 |
| ATOM | 816 | | AS | P A1107 | 17.446 | | | 1.00 30. | | N |
| ATOM | 817 | | | P A1107 | 17.878 | 29.789 | 4.392 | 1.00 31. | 74 | С |

| ATOM | 818 | СВ | ASP | A1107 | 18.324 | 28.992 | 3.160 | 1.00 33.44 | С |
|--------------|------------|---------|-------|----------------|------------------|------------------|----------------|--------------------------|--------|
| ATOM | 819 | CG | ASP | A1107 | 19.499 | 28.054 | 3.454 | 1.00 35.18 | С |
| ATOM | 820 | OD1 | ASP | A1107 - | 19.827 | 27.214 | 2.582 | 1.00 36.15 | 0 . |
| MOTA | 821 | OD2 | ASP | A1107 | 20.099 | 28.153 | 4.548 | 1.00 35.79 | 0 |
| MOTA | 822 | | | A1107 | 16.720 | 30.722 | 4.020 | 1.00 31.63 | С |
| MOTA | 823 | 0 | ASP | A1107 | 16.913 | 31.724 | 3.334 | 1.00 31.90 | 0 |
| MOTA | 824 | | | A1108 | 15.518 | 30.401 | 4.494 | 1.00 31.41 | Ŋ |
| MOTA | 825 | | | A1108 | 14.336 | 31.201 | 4.175 | 1.00 30.98 | C |
| ATOM | 826 | CB | GLN | A1108 | 13.340 | 30.345 | 3.399 | 1.00 32.64 | C |
| MOTA | 827 | CG | | A1108 | 13.860 | 29.898 | 2.038 | 1.00 34.63 | C |
| ATOM | 828 | | | A1108 | 12.917 | 28.945 | 1.346 | 1.00 35.98 | . C |
| ATOM | 829 | | | A1108 | 12.698 | 27.819 | 1.807 | 1.00 36.85 | 0 |
| ATOM | 830 | NE2 | | A1108 | 12.340 | 29.391 | 0.231 | 1.00 36.81 | N |
| ATOM | 831 | C | | A1108 | 13.616 | 31.862 | 5.338 | 1.00 29.94 | C 0 |
| MOTA | 832 | 0 | | A1108 | 12.985 | 32.899 | 5.158 | 1.00 29.44 | |
| MOTA | 833 | N | | A1109 | 13.700 | 31.269 | 6.529 | 1.00 29.06 | N C |
| MOTA | 834 | CA | | A1109 | 13.024 | 31.838 | 7.692 | 1.00 27.73 | c |
| MOTA | 835 | СВ | | A1109 | 11.762 | 31.036 | 8.037 | 1.00 27.57 | C |
| ATOM | 836 | CG | | A1109 | 10.744 | 31.005 | 6.941 | 1.00 27.23 | C |
| MOTA | 837 | | | A1109 | 10.788 | 30.017 | 5.962 | 1.00 27.53 1.00 27.16 | C |
| MOTA | 838 | | | A1109 | 9.749 | 31.976 | 6.871 | 1.00 27.10 | c |
| ATOM | 839 | | | A1109 | 9.852 | 30.000 | 4.921 | 1.00 27.28 | C |
| ATOM | 840 | | | A1109 | 8.810 | 31.970 | 5.838 | 1.00 26.77 | č |
| ATOM | 841 | CZ | | A1109 | 8.861 | 30.981 | 4.861 | 1.00 26.95 | č |
| MOTA | 842 | С | | A1109 | 13.868 | 31.932 31.243 | 8.950 9.102 | 1.00 20.93 | ő |
| ATOM | 843 | 0 | | A1109 | 14.877 | | 9.852 | 1.00 27.13 | N |
| ATOM | 844 | N | | A1110 | 13.431 | 32.803 | 11.138 | 1.00 25.13 | C |
| ATOM | 845 | CA | | A1110 | 14.080 | 32.992 34.347 | 11.138 | 1.00 25.40 | Č |
| ATOM | 846 | CB | | A1110 | 14.844 | 35.510 | 11.197 | 1.00 25.40 | Č |
| MOTA | 847 | | | A1110 | 13.874 | 34.449 | 12.499 | 1.00 25.77 | Č |
| MOTA | 848 | | | A1110 | 15.623 12.956 | 32.973 | 12.184 | 1.00 24.39 | Č |
| ATOM | 849 | C | | A1110 | 11.863 | 33.500 | 11.936 | 1.00 24.33 | Ō |
| MOTA | 850 | 0 | | A1110 A1111 | 13.206 | 32.344 | 13.332 | 1.00 23.30 | N |
| ATOM | 851 852 | N CA | | A1111 | 12.208 | 32.289 | 14.404 | 1.00 22.55 | С |
| ATOM ATOM | 853 | CB | | A1111 | 11.610 | 30.888 | 14.562 | 1.00 22.93 | С |
| ATOM | 854 | OG1 | | A1111 | 12.670 | 29.954 | 14.786 | 1.00 24.79 | 0 |
| ATOM | 855 | | | A1111 | 10.839 | 30.479 | 13.323 | 1.00 23.61 | С |
| ATOM | 856 | C C | | A1111 | 12.830 | 32.664 | 15.746 | 1.00 21.62 | С |
| MOTA | 857 | Ö | | A1111 | 13.999 | 32.377 | 16.002 | 1.00 21.64 | 0 |
| MOTA | 858 | N | | A1112 | 12.041 | 33.299 | 16.605 | 1.00 20.37 | N |
| MOTA | 859 | CA | | A1112 | 12.522 | 33.688 | 17.922 | 1.00 19.66 | С |
| ATOM | 860 | СВ | | A1112 | 12.800 | 35.202 | 17.970 | 1.00 19.55 | С |
| ATOM | 861 | C | | A1112 | 11.516 | 33.311 | 19.004 | 1.00 19.07 | С |
| ATOM | 862 | Ö | | A1112 | 10.302 | 33.410 | 18.814 | 1.00 19.29 | 0 |
| MOTA | 863 | N | | A1113 | 12.034 | 32.872 | 20.139 | 1.00 17.99 | N |
| ATOM | 864 | CA | | R A1113 | 11.195 | 32.506 | 21.263 | 1.00 17.22 | C |
| ATOM | 865 | СВ | | R A1113 | 11.174 | 30:989 | 21.457 | 1.00 16.88 | С |
| ATOM | 866 | OG | | R A1113 | 10.313 | 30.614 | 22.521 | 1.00 16.26 | 0 |
| ATOM | 867 | C | | R A1113 | 11.782 | 33.180 | 22.487 | 1.00 17.09 | С |
| ATOM | 868 | 0 | | R A1113 | 12.995 | 33.112 | 22.733 | 1.00 16.32 | 0 |
| ATOM | 869 | N | | A1114 | 10.906 | 33.831 | 23.245 | 1.00 17.10 | N |
| ATOM | 870 | CA | VAI | A1114 | 11.289 | 34.548 | 24.451 | 1.00 16.74 | C |
| MOTA | 871 | CB | VAI | A1114 | 11.164 | | 24.243 | | C |
| ATOM | 872 | CG1 | . VAI | L A1114 | 11.205 | | 25.592 | | . C |
| ATOM | 873 | CG2 | | A1114 | 12.298 | | 23.329 | | C |
| MOTA | 874 | С | VAI | L A1114 | 10.422 | 34.149 | 25.635 | 1.00 17.36 | С |
| | | | | | | | | | |

| ATOM | 875 | 0 | VAL | A1114 | 9.190 | | 25.544 | 1.00 16.90 | 0 |
|------|-----|-----|-------|---------|--------|------------------|--------|--------------------------|-----|
| ATOM | 876 | N | ILE | A1115 | 11.073 | 33.834 | 26.747 | 1.00 17.78 | N |
| ATOM | 877 | | | A1115 | 10.354 | 33.478 | 27.957 | 1.00 18.59 | С |
| ATOM | 878 | | | A1115 | 10.632 | 32.020 | 28.395 | 1.00 17.89 | С |
| ATOM | 879 | | | A1115 | 9.806 | 31.691 | 29.641 | 1.00 17.73 | , с |
| ATOM | 880 | | | A1115 | 10.247 | 31.053 | 27.272 | 1.00 18.13 | С |
| ATOM | 881 | | | A1115 | 10.654 | 29.599 | 27.521 | 1.00 17.22 | С |
| ATOM | 882 | C | | A1115 | 10.830 | 34.431 | 29.049 | 1.00 19.32 | С |
| ATOM | 883 | | | A1115 | 12.025 | 34.538 | 29.304 | 1.00 19.25 | 0 |
| ATOM | 884 | | | A1116 | 9.895 | 35.137 | 29.670 | 1.00 20.62 | N |
| | | CA | | A1116 | 10.239 | 36.066 | 30.736 | 1.00 22.56 | С |
| ATOM | 885 | | | A1116 | 9.408 | 37.341 | 30.617 | 1.00 22.06 | С |
| ATOM | 886 | | | A1116 | 9.547 | 38.064 | 29.272 | 1.00 22.11 | С |
| ATOM | 887 | CG | | A1116 | 8.540 | 39.207 | 29.187 | 1.00 21.22 | С |
| ATOM | 888 | | | | 10.969 | 38.578 | 29.113 | 1.00 21.72 | Ċ |
| MOTA | 889 | | | A1116 | 9.984 | 35.379 | 32.069 | 1.00 24.06 | C |
| MOTA | 890 | C | | A1116 | 8.936 | 34.765 | 32.275 | 1.00 23.78 | 0 |
| MOTA | 891 | 0 | | A1116 | | 35.486 | 32.970 | 1.00 25.93 | N |
| MOTA | 892 | N | | A1117 | 10.953 | | 34.267 | | C |
| MOTA | 893 | CA | | A1117 | 10.857 | 34.843 33.502 | 34.207 | 1.00 28.05 | Č |
| ATOM | 894 | СВ | | A1117 | 11.604 | | 35.536 | 1.00 28.32 | Č |
| MOTA | 895 | CG | | A1117 | 11.800 | 32.793 | | 1.00 28.66 | Č |
| MOTA | 896 | CD | | A1117 | 12.626 | 31.512 | 35.405 | 1.00 28.33 | 0 |
| MOTA | 897 | | | A1117 | 13.711 | 31.567 | 34.777 | | 0 |
| MOTA | 898 | OE2 | | A1117 | 12.196 | 30.458 | 35.936 | 1.00 28.07 1.00 29.70 | Č |
| ATOM | 899 | С | | A1117 | 11.413 | 35.699 | 35.404 | | 0 |
| MOTA | 900 | 0 | | A1117 | 12.242 | 36.583 | 35.190 | 1.00 29.81 | |
| ATOM | 901 | N | | A1118 | 10.928 | 35.441 | 36.615 | 1.00 31.64 | N |
| ATOM | 902 | CA | GLU | A1118 | 11.416 | 36.141 | 37.794 | 1.00 33.73 | C |
| ATOM | 903 | CB | | A1118 | 10.860 | 37.567 | 37.862 | 1.00 35.16 | C |
| ATOM | 904 | CG | | A1118 | 9.358 | 37.670 | 37.941 | 1.00 37.05 | C |
| MOTA | 905 | CD | | A1118 | 8.900 | 39.113 | 38.056 | 1.00 38.65 | |
| ATOM | 906 | OE1 | GLU | A1118 | 9.476 | 39.973 | | 1.00 38.82 | 0 |
| MOTA | 907 | OE2 | GLU | A1118 | 7.961 | 39.385 | 38.848 | 1.00 39.77 | 0 |
| ATOM | 908 | С | GLU | A1118 | 11.043 | 35.365 | 39.048 | 1.00 34.16 | C |
| MOTA | 909 | 0 | GLU | A1118 | 9.912 | 34.845 | 39.107 | 1.00 34.38 | 0 |
| ATOM | 910 | TXO | GLU | A1118 | 11.894 | 35.280 | 39.956 | 1.00 35.21 | 0 |
| TER | 911 | | GLU | A1118 | | | | | |
| MOTA | 912 | CB | MET | B2003 | 5.244 | 24.216 | 39.082 | 1.00 30.13 | C |
| MOTA | 913 | CG | MET | B2003 | 5.229 | 22,763 | 38.655 | 1.00 32.03 | C |
| ATOM | 914 | SD | MET | B2003 | 4.499 | 21.640 | 39.877 | 1.00 34.60 | S |
| ATOM | 915 | CE | MET | B2003 | 5.729 | 20.323 | 39.875 | 1.00 32.91 | С |
| ATOM | 916 | С | MET | B2003 | 5.364 | 24.946 | 36.697 | 1.00 27.68 | C |
| MOTA | 917 | 0 | MET | B2003 | 4.190 | 25.254 | 36.454 | 1.00 27.76 | 0 |
| ATOM | 918 | N | MET | B2003 | 5.824 | 26.555 | 38.533 | 1.00 28.66 | N |
| ATOM | 919 | CA | MET | B2003 | 5.954 | 25.143 | 38.090 | 1.00 28.51 | С |
| ATOM | 920 | N | ILE | E B2004 | 6.184 | 24.439 | 35.782 | 1.00 26.12 | N |
| ATOM | 921 | CA | ILE | E B2004 | 5.730 | 24.192 | 34.423 | 1.00 24.36 | С |
| ATOM | 922 | CB | ILE | E B2004 | 6.907 | 24:200 | 33.423 | | C |
| ATOM | 923 | CG2 | : ILE | E B2004 | 6.445 | 23.691 | 32.062 | | C |
| ATOM | 924 | | | E B2004 | 7.465 | 25.624 | 33.300 | | C |
| MOTA | 925 | | | E B2004 | 8.670 | | 32.379 | | . С |
| MOTA | 926 | | ILE | E B2004 | 5.035 | 22.841 | 34.376 | | C |
| ATOM | 927 | | IL | E B2004 | 5.537 | | 34.917 | | 0 |
| ATOM | 928 | | VA | L B2005 | 3.866 | 22.793 | | | N |
| ATOM | 929 | | | L B2005 | 3.151 | 21.530 | 33.660 | | C |
| ATOM | 930 | | VA: | L B2005 | 1.853 | 21.564 | 34.494 | | C |
| ATOM | 931 | | | L B2005 | 2.204 | | 35.959 | 1.00 21.47 | С |
| 0 | | | | | | | | | |

| | | | | | | | | | and the second s |
|------|-----|------|-----|---------|-------|-----------------------|----------|------------|--|
| ATOM | 932 | CG2 | VAL | B2005 | 0.920 | | 33.994 | 1.00 21.79 | . C |
| MOTA | 933 | С | VAL | B2005 | 2.847 | 7 21.133 | 32.228 | 1.00 22.00 | C |
| MOTA | 934 | 0 | VAL | B2005 | 2.130 | 20.163 | 31.995 | 1.00 22.54 | 0 |
| ATOM | 935 | N | GLY | B2006 | 3.417 | 7 21.880 | 31.278 | 1.00 21.53 | N |
| ATOM | 936 | CA | GLY | B2006 | 3.225 | 5 21.594 | 29.867 | 1.00 20.47 | С |
| ATOM | 937 | С | GLY | B2006 | 3.802 | 22.634 | 28.914 | 1.00 19.98 | С |
| ATOM | 938 | 0 | GLY | B2006 | 3.873 | 3 23.820 | 29.237 | 1.00 20.12 | 0 |
| ATOM | 939 | | | B2007 | 4.23 | 5 22.175 | 27.741 | 1.00 19.33 | N |
| ATOM | 940 | | | B2007 | 4.789 | 9 23.031 | 26.686 | 1.00 18.80 | С |
| ATOM | 941 | | | B2007 | 6.30 | 23.191 | 26.832 | 1.00 18.37 | С |
| ATOM | 942 | CG | HIS | B2007 | 6.94 | 5 23.945 | 25.708 | 1.00 18.59 | C |
| ATOM | 943 | CD2 | HIS | B2007 | 8.08 | 8 23.712 | 25.015 | 1.00 19.30 | С |
| ATOM | 944 | ND1 | HIS | B2007 | 6.44 | 7 25.138 | 25.226 | 1.00 18.65 | N |
| ATOM | 945 | | | B2007 | 7.25 | 4 25.607 | 24.289 | 1.00 18.01 | С |
| ATOM | 946 | | | B2007 | 8.25 | 9 24.763 | 24.143 | 1.00 18.26 | N |
| ATOM | 947 | C | | B2007 | 4.48 | 2 22.387 | 25.342 | 1.00 18.69 | С |
| ATOM | 948 | 0 | | B2007 | 4.73 | 1 21.197 | 25.146 | 1.00 17.82 | 0 |
| ATOM | 949 | N | | B2008 | 3.92 | 5 23.174 | 24.425 | 1.00 19.16 | N |
| ATOM | 950 | CA | | B2008 | 3.59 | 9 22.655 | 23.110 | 1.00 18.31 | С |
| ATOM | 951 | С | | B2008 | 3.70 | 3 23.724 | 22.043 | 1.00 18.66 | |
| ATOM | 952 | Ō | | B2008 | 3.37 | 8 24.890 | 22.297 | 1.00 18.62 | Ó |
| ATOM | 953 | N | ILE | B2009 | 4.17 | 5 23.336 | 20.858 | 1.00 18.18 | N |
| MOTA | 954 | CA | ILE | B2009 | 4.28 | 2 24.257 | 19.736 | 1.00 18.56 | |
| ATOM | 955 | CB | | B2009 | 5.74 | 7 24.562 | 19.351 | 1.00 18.23 | |
| ATOM | 956 | CG2 | | B2009 | 6.47 | 1 25.174 | 20.538 | 1.00 17.94 | С |
| ATOM | 957 | | ILE | B2009 | 6.44 | 0 23.285 | 18.847 | 1.00 17.91 | |
| ATOM | 958 | | | B2009 | 7.81 | 9 23.525 | 18.220 | 1.00 16.62 | C |
| MOTA | 959 | C | | B2009 | 3.60 | 1 23.657 | 18.513 | 1.00 19.50 | |
| ATOM | 960 | 0 | | B2009 | 3.28 | 6 22.470 | 18.472 | 1.00 18.95 | 0 |
| ATOM | 961 | N | | B2010 | 3.35 | 6 24.492 | 17.518 | 1.00 20.39 | |
| ATOM | 962 | CA | | B2010 | 2.75 | 1 24.015 | 16.298 | 1.00 21.57 | |
| ATOM | 963 | CB · | | B2010 | 1.25 | 1 23.773 | 3 16.481 | 1.00 22.40 | |
| ATOM | 964 | CG | ASP | B2010 | 0.63 | 35 22.980 | 15.317 | 1.00 23.74 | C |
| MOTA | 965 | OD1 | ASP | B2010 | 0.22 | 23.595 | 14.308 | 1.00 23.88 | |
| ATOM | 966 | OD2 | ASP | B2010 | 0.57 | 6 21.731 | 15.415 | 1.00 24.74 | |
| MOTA | 967 | С | ASP | B2010 | 2.97 | 79 25.019 | 9 15.200 | 1.00 22.11 | |
| ATOM | 968 | 0 | ASP | B2010 | 3.03 | 32 26.224 | 15.443 | 1.00 22.03 | |
| ATOM | 969 | N | ILE | B2011 | 3.14 | 15 24.502 | 2 13.991 | 1.00 23.00 | |
| MOTA | 970 | CA | ILE | B2011 | 3.33 | 35 25.33 (| 6 12.824 | 1.00 24.24 | |
| ATOM | 971 | CB | ILE | B2011 | 4.81 | L8 25.320 | 12.339 | 1.00 24.43 | |
| ATOM | 972 | CG2 | ILE | B2011 | 5.25 | 58 23.905 | 5 11.972 | 1.00 24.62 | |
| MOTA | 973 | CG1 | ILE | B2011 | 4.97 | 70 26.24 | 4 11.133 | 1.00 25.18 | |
| MOTA | 974 | CD1 | ILE | B2011 | 6.4 | 26.43 | | 1.00 26.49 | |
| ATOM | 975 | С | ILE | B2011 | 2.39 | | | 1.00 25.03 | |
| MOTA | 976 | 0 | ILE | B2011 | 2.25 | | | | |
| MOTA | 977 | N | GLU | B2012 | 1.73 | | | 1.00 26.1 | |
| MOTA | 978 | CA | GLU | B2012 | 0.83 | | | | |
| ATOM | 979 | CB | GLU | B2012 | -0.6 | 36 25:69 | | 1.00 28.0 | 6 C |
| ATOM | 980 | CG | GLU | J B2012 | -1.1 | | | 1.00 30.3 | |
| MOTA | 981 | CD | GLU | J B2012 | -1.2 | | | 1.00 31.8 | |
| MOTA | 982 | | | J B2012 | -1.4 | | | | |
| MOTA | 983 | OE2 | GLU | J B2012 | -1.0 | | | 1.00 31.8 | |
| ATOM | 984 | С | GLt | J B2012 | 1.1 | | | 1.00 27.0 | |
| MOTA | 985 | 0 | | J B2012 | 1.5 | | | | |
| MOTA | 986 | N | | J B2013 | 0.9 | | | | |
| MOTA | 987 | | | J B2013 | 1.1 | | | | |
| MOTA | 988 | CB | GL | J B2013 | 1.5 | 33 25.01 | 8 5.253 | 1.00 28.0 | 6 C |
| | | | | | | | | | |

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|--------------|--------------|--------|-----|---------|--------|-----------|--------|--------------|---|
| ATOM | 989 | CG | GLU | B2013 | 1.806 | 5 25.553 | 3.851 | 1.00 29.06 | C |
| ATOM | 990 | CD | GLU | B2013 | 2.105 | 5 24.447 | 2.858 | 0.05 28.78 | С |
| MOTA | 991 | OE1 | GLU | B2013 | 3.074 | 23.691 | 3.081 | 0.05 28.87 | 0 |
| ATOM | 992 | OE2 | GLU | B2013 | 1.370 | 24.335 | 1.856 | 0.05 28.90 | 0 |
| ATOM | 993 | С | GLU | B2013 | -0.268 | 3 26.626 | 5.939 | 1.00 27.67 | С |
| ATOM | 994 | | | B2013 | -1.250 | 25.894 | 5.982 | 1.00 27.29 | 0 |
| ATOM | 995 | _ | | B2014 | -0.350 | | 5.644 | 1.00 28.07 | N |
| ATOM | 996 | CA | | B2014 | -1.62 | | 5.330 | 1.00 28.65 | С |
| | 997 | CB | | B2014 | -1.42 | | 4.986 | 1.00 28.56 | С |
| ATOM | | | | B2014 | -1.33 | | 6.147 | 1.00 28.97 | С |
| MOTA | 998 | | | | -2.67 | | 6.840 | 1.00 28.76 | С |
| ATOM | 999. | | | B2014 | -0.26 | | 7.139 | 1.00 28.89 | Ċ |
| ATOM | 1000 | | | B2014 | | | 4.189 | 1.00 28.89 | Č |
| ATOM | 1001 | С | | B2014 | -2.35 | | | 1.00 28.92 | Ö |
| MOTA | 1002 | 0 | | B2014 | -3.58 | | 4.189 | 1.00 29.40 | N |
| ATOM | 1003 | N | | B2015 | -1.58 | | 3.228 | | C |
| ATOM | 1004 | CA | | B2015 | -2.13 | | 2.058 | 1.00 29.93 | C |
| MOTA | 1005 | CB | ALA | B2015 | -0.99 | | 1.146 | 1.00 29.23 | |
| ATOM | 1006 | С | ALA | B2015 | -3.03 | | 2.401 | 1.00 30.15 | С |
| MOTA | 1007 | 0 | ALA | B2015 | -4.06 | | 1.760 | 1.00 30.32 | 0 |
| ATOM | 1008 | N | SER | B2016 | -2.64 | | 3.403 | 1.00 30.53 | N |
| ATOM | 1009 | CA | SER | B2016 | -3.44 | 5 23.544 | 3.776 | 1.00 31.47 | C |
| ATOM | 1010 | CB | SER | B2016 | -2.62 | 5 22.583 | 4.640 | 1.00 31.89 | С |
| ATOM | 1011 | OG | SER | B2016 | -2.22 | 9 23.193 | 5.846 | 1.00 33.02 | 0 |
| ATOM | 1012 | С | | B2016 | -4.73 | 5 23.946 | 4.487 | 1.00 31.84 | С |
| ATOM | 1013 | Ō | SER | B2016 | -5.74 | 1 23.243 | 4.391 | 1.00 31.71 | 0 |
| ATOM | 1014 | N | | B2017 | -4.71 | 6 25.068 | 5.201 | 1.00 32.07 | N |
| ATOM | 1015 | CA | | B2017 | -5.93 | | 5.861 | 1.00 32.52 | С |
| ATOM | 1016 | CB | | B2017 | -5.65 | | 6.843 | 1.00 32.37 | С |
| ATOM | 1017 | | | B2017 | -6.97 | | | 1.00 32.53 | С |
| ATOM | 1018 | | | B2017 | -4.75 | | | 1.00 32.12 | С |
| MOTA | 1019 | | | B2017 | -5.39 | | | 1.00 31.06 | C |
| ATOM | 1020 | C | | B2017 | -6.86 | | | 1.00 33.04 | С |
| ATOM | 1021 | 0 | | B2017 | -8.08 | | | 1.00 32.69 | 0 |
| ATOM | 1021 | N | | B2018 | -6.26 | _ | | 1.00 33.86 | N |
| | 1022 | CA | | B2018 | -7.00 | | | | С |
| MOTA MOTA | 1023 | CB | | B2018 | -6.04 | | | | С |
| | 1024 | CG | | B2018 | -5.54 | | | | C |
| ATOM | 1025 | CD | | J B2018 | -6.55 | | | | С |
| ATOM | 1026 | | | J B2018 | -7.6 | | | | 0 |
| ATOM | 1027 | | | J B2018 | -6.23 | | | | 0 |
| ATOM | | C | | J B2018 | -7.78 | | | | С |
| ATOM | 1029 1030 | | | J B2018 | -8.9 | | | | 0 |
| ATOM | 1030 | О N | | R B2019 | -7.0 | | | | N |
| ATOM | | CA | | R B2019 | -7.7 | | | | С |
| ATOM | 1032 | CB | | R B2019 | | 39 22.610 | | | С |
| ATOM | | | | R B2019 | -5.7 | | | | 0 |
| ATOM | 1034 | OG | | R B2019 | -8.7 | | | | С |
| ATOM | 1035 | С | | | -9.8 | | | | 0 |
| ATOM | 1036 | | | R B2019 | -8.4 | | | | Ŋ |
| ATOM | 1037 | | | A B2020 | -9.3 | | | | C |
| ATOM | 1038 | | | A B2020 | | | | | C |
| ATOM | 1039 | | | A B2020 | -8.8 | | | | Č |
| MOTA | 1040 | | | A B2020 | -10.7 | | | | Õ |
| MOTA | 1041 | | | A B2020 | -11.7 | | | | И |
| MOTA | 1042 | | | L B2021 | -10.6 | | | | C |
| MOTA | 1043 | | | L B2021 | -11.7 | | | | Č |
| ATOM | 1044 | | | L B2021 | -11.4 | | | | č |
| MOTA | 1045 | CG | T A | L B2021 | -12.6 | 08 27.73 | 2 3.88 | ± 1.00 34.73 | C |

| ATOM | 1046 | CG2 | VAL | B2021 | -10.9 | 51 | 27.136 | 5.63 | 7 1.00 | 35.33 | С |
|------|------|-----|-----|-------|-------|-------|--------|-------|---------|-------|---|
| ATOM | 1047 | С | | B2021 | -12.5 | | 25.174 | 2.75 | | 36.00 | С |
| ATOM | 1048 | ō | | B2021 | -13.7 | | 24.985 | 2.74 | | 35.93 | Ō |
| ATOM | 1049 | N | | B2022 | -11.7 | | 25.237 | 1.64 | | 36.68 | N |
| ATOM | 1050 | CA | | B2022 | -12.4 | | 25.072 | | 6 1.00 | | C |
| | | | | | | | | | | | C |
| ATOM | 1051 | CB | | B2022 | -11.3 | | 25.211 | -0.81 | | 38.05 | |
| ATOM | 1052 | | | B2022 | -10.8 | | 26.549 | -0.83 | | 37.71 | 0 |
| ATOM | 1053 | | | B2022 | -11.9 | | 24.898 | -2.16 | | 37.87 | С |
| ATOM | 1054 | С | | B2022 | -13.0 | | 23.701 | 0.21 | | 38.58 | С |
| ATOM | 1055 | 0 | | B2022 | -14.2 | 204 | 23.584 | -0.23 | 4 1.00 | 38.63 | 0 |
| ATOM | 1056 | N | ARG | B2023 | -12.3 | 348 | 22.666 | 0.62 | 9 1.00 | 39.65 | N |
| ATOM | 1057 | CA | ARG | B2023 | -12.8 | 64 | 21.306 | 0.56 | 3 1.00 | 41.03 | С |
| MOTA | 1058 | CB | ARG | B2023 | -11.8 | 328 | 20.317 | 1.10 | 6 1.00 | 41.66 | C |
| ATOM | 1059 | CG | ARG | B2023 | -11.8 | 391 | 18.939 | 0.45 | 2 1.00 | 43.04 | C |
| ATOM | 1060 | CD | ARG | B2023 | -13.3 | | 18.416 | 0.39 | 5 1.00 | 43.90 | С |
| ATOM | 1061 | NE | | B2023 | -13.4 | | 17.090 | -0.20 | | 44.75 | N |
| ATOM | 1062 | CZ | | B2023 | -14.5 | | 16.371 | -0.23 | | 45.34 | С |
| ATOM | 1063 | | | B2023 | -15.6 | | 16.862 | 0.30 | | 45.03 | N |
| ATOM | 1064 | | | B2023 | -14.5 | | 15.157 | -0.77 | | 45.61 | N |
| ATOM | 1065 | C | | B2023 | -14.1 | | 21.138 | 1.34 | | 41.52 | C |
| | 1066 | | | B2023 | -15.1 | | 20.712 | 0.78 | | 41.49 | 0 |
| ATOM | | 0 | | | -14.1 | | | | | | |
| ATOM | 1067 | N | | B2024 | | | 21.467 | 2.63 | | 41.94 | N |
| ATOM | 1068 | CA | | B2024 | -15.2 | | 21.343 | 3.51 | | 42.45 | C |
| ATOM | 1069 | CB | | B2024 | -14.9 | | 20.424 | 4.67 | | 43.39 | С |
| ATOM | 1070 | CG | | B2024 | -14.5 | | 19.050 | 4.25 | | 44.50 | C |
| MOTA | 1071 | | | B2024 | -13.2 | | 18.468 | 4.19 | | 44.72 | С |
| ATOM | 1072 | | | B2024 | -15.4 | | 18.115 | 3.77 | | 45.05 | N |
| MOTA | 1073 | | | B2024 | -14.7 | 758 | 17.018 | 3.43 | 1.00 | 45.22 | С |
| MOTA | 1074 | NE2 | HIS | B2024 | -13.4 | 173 | 17.206 | 3.67 | 7 1.00 | 45.24 | N |
| MOTA | 1075 | С | HIS | B2024 | -15.7 | 713 ' | 22.697 | 4.04 | 10 1.00 | 42.58 | С |
| MOTA | 1076 | 0 | HIS | B2024 | -14.9 | 934 | 23.412 | 4.67 | 2 1.00 | 42.87 | 0 |
| ATOM | 1077 | N | GLU | B2025 | -16.9 | 967 | 23.050 | 3.78 | 1.00 | 42.39 | N |
| MOTA | 1078 | CA | GLU | B2025 | -17.4 | 190 | 24.326 | 4.24 | 2 1.00 | 41.91 | С |
| MOTA | 1079 | CB | GLU | B2025 | -18.7 | 732 | 24.732 | 3.43 | 37 1.00 | 43.59 | С |
| MOTA | 1080 | CG | GLU | B2025 | -18. | 797 | 26.229 | 3.19 | 3 1.00 | 45.80 | С |
| MOTA | 1081 | CD | GLU | B2025 | -20.3 | | 26.675 | 2.5 | 4 1.00 | 47.26 | С |
| ATOM | 1082 | OE1 | | B2025 | -20.6 | | 26.003 | 1.60 | | 47.52 | 0 |
| MOTA | 1083 | | | B2025 | -20.6 | | 27.710 | 3.00 | | 48.07 | 0 |
| ATOM | 1084 | C | | B2025 | -17.8 | | 24.211 | 5.7 | | 40.39 | Ċ |
| ATOM | 1085 | 0 | | B2025 | -18. | | 25.203 | 6.3 | | 40.62 | 0 |
| ATOM | 1086 | N | | B2026 | -17. | | 22.993 | 6.2 | | 38.87 | N |
| ATOM | 1087 | CA | | B2026 | -18. | | 22.788 | 7.63 | | 36.84 | C |
| ATOM | 1088 | C | | B2026 | -16.8 | | 22.836 | 8.50 | | 35.50 | Č |
| ATOM | 1089 | Ö | | B2026 | -16. | | 22.961 | 9.73 | | 35.89 | Õ |
| ATOM | 1090 | N | | B2027 | -15. | | 22.746 | 7.8 | | 33.86 | N |
| MOTA | 1091 | CA | | B2027 | | | | | | 32.08 | C |
| | | | | | -14. | | | | | | |
| ATOM | 1092 | CB | | B2027 | -13.3 | | 22.958 | 7.5 | | 31.28 | C |
| ATOM | 1093 | CG | | B2027 | -11. | | 22:896 | 8.1 | | 29.92 | C |
| ATOM | 1094 | | | B2027 | -11. | | 21.682 | 8.5 | | 28.97 | C |
| ATOM | 1095 | | | B2027 | -11. | | 24.054 | 8.2 | | 29.17 | C |
| ATOM | 1096 | | | B2027 | -10. | | 21.623 | 9.1 | | 28.66 | С |
| ATOM | 1097 | | | B2027 | -9. | | 24.006 | 8.8 | | 28.77 | С |
| MOTA | 1098 | CZ | | B2027 | -9. | | 22.790 | 9.2 | | 28.68 | С |
| ATOM | 1099 | C, | | B2027 | -14. | | 23.801 | 9.6 | | 31.46 | С |
| ATOM | 1100 | 0 | | B2027 | -14. | | 23.465 | 10.8 | | 31.23 | 0 |
| MOTA | 1101 | N | | B2028 | -14. | | 25.067 | 9.2 | | 30.51 | N |
| ATOM | 1102 | CA | ALA | B2028 | -14. | 360 | 26.169 | 10.2 | 28 1.00 | 30.25 | С |
| | | | | | | | | | | | |

| ATOM | 1103 | CB | ALA | B2028 | -14.624 | 27.487 | 9.517 | 1.00 30.53 | С |
|-------|------|----------|------|-------|--------------------|--------|------------------|------------|--------|
| ATOM | 1104 | С | | B2028 | -15.305 | 26.030 | 11.421 | 1.00 30.13 | C |
| MOTA | 1105 | 0 | | B2028 | -14.926 | 26.308 | 12.561 | 1.00 29.80 | 0 |
| ATOM | 1106 | N | | B2029 | -16.533 | 25.600 | 11.160 | 1.00 30.02 | N |
| ATOM | 1107 | CA | | B2029 | -17.520 | 25.448 | 12.225 | 1.00 30.10 | C |
| ATOM | 1108 | CB | | B2029 | -18.882 | 25.053 | 11.637 | 1.00 30.49 | č |
| ATOM | 1109 | CG | | B2029 | -19.552 | 26.148 | 10.821 | 1.00 31.20 | č |
| ATOM | 1110 | CD | | B2029 | -20.765 | 25.618 | 10.074 | 0.05 30.87 | č |
| ATOM | 1111 | | | B2029 | -21.354 | 26.675 | 9.153 | 0.05 30.89 | Ċ |
| ATOM | 1112 | CE NZ | | B2029 | -22.504 | 26.150 | 8.365 | 0.05 30.76 | N |
| | 1113 | | | B2029 | -17.099 | 24.408 | 13.248 | 1.00 29.50 | C |
| MOTA | | С | | | | | | 1.00 29.99 | |
| MOTA | 1114 | 0 | | B2029 | -17.467 -16.326 | 24.491 | 14.420 12.798 | 1.00 29.99 | O N |
| ATOM | 1115 | N | | B2030 | | 23.428 | | | |
| ATOM | 1116 | CA | | B2030 | -15.877 | 22.348 | 13.667 | 1.00 27.83 | C |
| ATOM | 1117 | CB | | B2030 | -15.616 | 21.093 | 12.822 | 1.00 27.88 | C |
| ATOM | 1118 | CG | | B2030 | -16.867 | 20.503 | 12.193 | 0.05 27.87 | C |
| MOTA | 1119 | CD. | | B2030 | -16.543 | 19.293 | 11.332 | 0.05 27.87 | C |
| MOTA | 1120 | NE | | B2030 | -15.748 | 19.648 | 10.160 | 0.05 27.89 | N |
| MOTA | 1121 | CZ | | B2030 | -15.379 | 18.785 | 9.218 | 0.05 27.88 | C |
| ATOM | 1122 | | | B2030 | -15.732 | 17.510 | 9.309 | 0.05 27.89 | N |
| MOTA | 1123 | NH2 | | B2030 | -14.658 | 19.196 | 8.184 | 0.05 27.87 | N |
| ATOM | 1124 | С | | B2030 | -14.631 | 22.698 | 14.477 | 1.00 26.83 | С |
| MOTA | 1125 | 0 | | B2030 | -14.391 | 22.134 | 15.541 | 1.00 26.57 | 0 |
| MOTA | 1126 | N | VAL | B2031 | -13.854 | 23.644 | 13.965 | 1.00 25.79 | N |
| ATOM | 1127 | CA | VAL | B2031 | -12.610 | 24.073 | 14.596 | 1.00 24.76 | С |
| MOTA | 1128 | CB | VAL | B2031 | -11.565 | 24.442 | 13.505 | 1.00 24.82 | С |
| ATOM | 1129 | CG1 | VAL | B2031 | -10.365 | 25.139 | 14.121 | 1.00 24.72 | С |
| ATOM | 1130 | CG2 | VAL | B2031 | -11.125 | 23.184 | 12.779 | 1.00 24.93 | C |
| MOTA | 1131 | С | VAL | B2031 | -12.806 | 25.263 | 15.523 | 1.00 23.81 | С |
| ATOM | 1132 | 0 | VAL | B2031 | -12.166 | 25.365 | 16.568 | 1.00 22.82 | 0 |
| MOTA | 1133 | N | LEU | B2032 | -13.709 | 26.149 | 15.127 | 1.00 23.54 | N |
| ATOM | 1134 | CA | LEU | B2032 | -13.997 | 27.361 | 15.873 | 1.00 23.22 | С |
| ATOM | 1135 | CB | LEU | B2032 | -14.157 | 28.528 | 14.893 | 1.00 22.85 | С |
| MOTA | 1136 | CG | LEU | B2032 | -12.924 | 28.789 | 14.022 | 1.00 22.24 | С |
| MOTA | 1137 | CDI | LEU | B2032 | -13.210 | 29.906 | 13.026 | 1.00 22.11 | С |
| MOTA | 1138 | CD2 | LEU | B2032 | -11.747 | 29.152 | 14.918 | 1.00 22.17 | С |
| ATOM | 1139 | С | LEU | B2032 | -15.233 | 27.256 | 16.744 | 1.00 23.32 | С |
| ATOM | 1140 | 0 | LEU | B2032 | -16.122 | 26.454 | 16.482 | 1.00 23.42 | 0 |
| MOTA | 1141 | N | | B2033 | -15.263 | 28.060 | 17.803 | 1.00 23.69 | N |
| ATOM | 1142 | CA | | B2033 | -16.404 | 28.105 | 18.713 | 1.00 23.81 | С |
| ATOM | 1143 | СВ | | B2033 | -16.002 | 28.538 | 20.129 | 1.00 23.49 | С |
| ATOM | 1144 | | | B2033 | -15.442 | 29.858 | 20.074 | 1.00 23.22 | 0 |
| ATOM | 1145 | CG2 | THR | B2033 | -15.004 | 27.571 | 20.726 | 1.00 22.82 | С |
| ATOM | 1146 | С | | B2033 | -17.312 | 29.191 | 18.162 | 1.00 24.17 | С |
| ATOM | 1147 | 0 | | B2033 | -16.915 | 29.930 | 17.264 | 1.00 24.05 | 0 |
| MOTA | 1148 | N | | B2034 | -18.516 | | | | N |
| MOTA | 1149 | CA | | B2034 | -19.456 | 30.322 | 18.246 | 1.00 25.88 | С |
| ATOM | 1150 | СВ | | B2034 | -20.704 | 30:326 | 19.127 | 1.00 25.52 | С |
| MOTA | 1151 | C | | B2034 | -18.793 | 31.704 | 18.245 | 1.00 26.34 | Ċ |
| ATOM | 1152 | Ō | | B2034 | -18.815 | 32.409 | 17.231 | 1.00 26.66 | 0 |
| ATOM | 1153 | N | | B2035 | -18.194 | 32.083 | 19.374 | 1.00 27.02 | N |
| ATOM | 1154 | CA | | B2035 | -17.518 | 33.375 | 19.477 | 1.00 27.85 | C |
| ATOM | 1155 | CB | | B2035 | -16.868 | 33.549 | 20.852 | 1.00 28.57 | Č |
| ATOM | 1156 | CG | | B2035 | -17.760 | 33.942 | 22.028 | 1.00 29.51 | C |
| ATOM | 1157 | | | B2035 | -16.879 | 34.241 | 23.246 | 1.00 29.47 | c |
| MOTA | 1158 | | | B2035 | -18.596 | 35.181 | 21.648 | 1.00 29.85 | C |
| ATOM | 1159 | C | | B2035 | -16.445 | 33.516 | 18.405 | 1.00 29.03 | c |
| ALOFI | 1100 | _ | טפיב | 22033 | 10.443 | 55.510 | 10.403 | 1.00 20.07 | C |

| ATOM ATOM ATOM | 1160 1161 | | | B2035 B2036 | -16.395 -15.578 | 34.516 32.518 | 17.687 18.308 | 1.00 2 1.00 2 | | 0 N |
|----------------------|--------------|----------|-----|----------------|--------------------|------------------|------------------|------------------|-------|--------|
| | | | GLU | B2036 | -15.578 | 32 518 | 18.308 | 1.00 2 | 7.90 | N |
| | | | | | | 32.310 | 10.500 | | | |
| | 1162 | CA | GLU | B2036 | -14.518 | 32.542 | 17.310 | 1.00 2 | | С |
| ATOM | 1163 | | | B2036 | -13.666 | 31.270 | 17.414 | 1.00 2 | | С |
| ATOM | 1164 | CG | GLU | B2036 | -12.568 | 31.339 | 18.474 | 1.00 2 | | C |
| ATOM | 1165 | CD | GLU | B2036 | -11.969 | 29.976 | 18.799 | 1.00 2 | | C |
| ATOM | 1166 | OE1 | GLU | B2036 | -10.797 | 29.925 | 19.226 | 1.00 2 | | 0 |
| ATOM | 1167 | OE2 | GLU | B2036 | -12.676 | 28.957 | 18.636 | 1.00 2 | | 0 |
| ATOM | 1168 | С | GLU | B2036 | -15.073 | 32.686 | 15.895 | 1.00 2 | | C |
| ATOM | 1169 | 0 | GLU | B2036 | -14.507 | 33.403 | 15.083 | 1.00 2 | | 0 |
| MOTA | 1170 | N | MET | B2037 | -16.169 | 31.990 | 15.604 | 1.00 2 | | N |
| ATOM | 1171 | CA | MET | B2037 | -16.800 | 32.038 | 14.283 | 1.00 3 | | C |
| MOTA | 1172 | CB | | B2037 | -17.984 | 31.069 | 14.211 | 1.00 3 | | C C |
| MOTA | 1173 | CG | | B2037 | -17.607 | 29.662 | 13.809 | 1.00 3 | | S |
| MOTA | 1174 | SD | | B2037 | -16.851 | 29.650 | 12.173 | 1.00 3 | | C |
| ATOM | 1175 | CE | | B2037 | -18.331 | 29.638 | 11.166 | 1.00 3 | | C |
| MOTA | 1176 | С | | B2037 | -17.286 | 33.436 | 13.934 | 1.00 | | 0 |
| MOTA | 1177 | 0 | | B2037 | -17.206 | 33.854 | 12.785 | 1.00 | | N |
| MOTA | 1178 | N | | B2038 | -17.789 | 34.153 | 14.934 | 1.00 | | C. |
| MOTA | 1179 | CA | | B2038 | -18.278 | 35.513 | 14.730 | 1.00 | | C |
| MOTA | 1180 | CB | | B2038 | -18.841 | 36.062 | 16.044 | 1.00 | | C |
| MOTA | 1181 | CG | | B2038 | -19.432 | 37.455 | 15.931 | 1.00 | | Č |
| ATOM | 1182 | CD | | B2038 | -20.528 | 37.714 | 16.955 | 1.00 | | ő |
| ATOM | 1183 | | | B2038 | -21.587 | 37.050 | 16.864 | 1.00 | | Ö |
| MOTA | 1184 | | | B2038 | -20.333 | 38.576 | 17.846 14.198 | 1.00 | | c |
| MOTA | 1185 | C | | B2038 | -17.163 | 36.418 | 13.397 | 1.00 | | Ö |
| ATOM | 1186 | 0 | | B2038 | -17.406 | 37.320 | 14.649 | 1.00 | | N |
| MOTA | 1187 | N | | B2039 | -15.936 | 36.181 36.972 | 14.179 | 1.00 | | C |
| ATOM | 1188 | CA | | B2039 | -14.810 -13.630 | 36.856 | 15.153 | 1.00 | | Č |
| MOTA | 1189 | CB | | B2039 | -12.370 | 37.601 | 14.720 | 1.00 | | Ċ |
| MOTA | 1190 | CG | | B2039 | -12.590 | 39.099 | 14.608 | 0.05 | | С |
| ATOM | 1191 | CD | | B2039 B2039 | -11.358 | 39.788 | 14.235 | | 35.24 | N |
| ATOM | 1192 | NE CZ | | B2039 | -11.260 | 41.099 | 14.040 | | 35.24 | С |
| ATOM | 1193 | | | B2039 | -10.095 | 41.634 | 13.703 | | 35.27 | N |
| ATOM | 1194 | | | B2039 | -12.325 | 41.875 | 14.182 | | 35.27 | N |
| MOTA | 1195 1196 | C | | B2039 | -14.418 | 36.445 | 12.797 | | 35.34 | С |
| MOTA MOTA | 1197 | Ö | | B2039 | -14.167 | 37.217 | 11.868 | 1.00 | 35.66 | 0 |
| ATOM | 1198 | N | | B2040 | -14.382 | 35.123 | 12.673 | 1.00 | 35.29 | N |
| ATOM | 1199 | CA | | B2040 | -14.042 | 34.473 | 11.414 | 1.00 | 35.77 | С |
| MOTA | 1200 | СВ | | B2040 | -14.241 | 32.961 | 11.545 | 1.00 | 34.55 | С |
| ATOM | 1201 | CG | | B2040 | -13.996 | 32.201 | 10.271 | | 33.98 | С |
| ATOM | 1202 | | PHE | E B2040 | -12.716 | 32.122 | 9.725 | 1.00 | 33.52 | С |
| ATOM | 1203 | CD2 | PHE | E B2040 | -15.045 | 31.564 | 9.614 | | 33.68 | C |
| ATOM | 1204 | | | E B2040 | -12.488 | 31.420 | 8.548 | | 33.41 | C |
| ATOM | 1205 | CE | PHE | E B2040 | -14.828 | 30.861 | 8.435 | | 33.27 | C |
| ATOM | 1206 | CZ | PHE | E B2040 | -13.549 | 30.787 | 7.899 | | 33.46 | С |
| ATOM | 1207 | | PHI | E B2040 | -14.916 | 34:997 | | | 36.68 | C |
| MOTA | 1208 | 0 | PHI | E B2040 | -14.445 | 35.199 | | | 36.38 | 0 |
| ATOM | 1209 | | THI | R B2041 | -16.191 | 35.221 | | | 37.87 | N |
| ATOM | 1210 | CA | | R B2041 | -17.121 | 35.692 | | | 39.25 | , C |
| MOTA | 1211 | CB | | R B2041 | -18.580 | 35.450 | | | 39.24 | C |
| ATOM | 1212 | | | R B2041 | -18.811 | 34.041 | | | 39.45 | O C |
| MOTA | | | | R B2041 | -19.540 | 36.001 | | | 40.16 | C |
| MOTA | | | | R B2041 | -16.947 | 37.159 | | | 39.72 | 0 |
| ATOM | | | | R B2041 | -17.496 | | | | 40.46 | N |
| ATOM | 1216 | 5 N | SE | R B2042 | -16.175 | 37.915 | 9.930 | 1.00 | 40.14 | 14 |

| ATOM | 1217 | CA | SER | B2042 | -15.970 | 39.327 | 9.609 | 1.00 | | C. |
|--------------|--------------|-----|-----|----------------|------------------|------------------|----------------|------|----------------|--------|
| MOTA | 1218 | CB | SER | B2042 | -16.159 | 40.184 | 10.858 | 1.00 | | С |
| MOTA | 1219 | OG | SER | B2042 | -17.449 | 39.989 | 11.399 | 1.00 | | 0 |
| ATOM | 1220 | | | B2042 | -14.588 | 39.596 | 9.033 | | 40.43 | C |
| MOTA | 1221 | 0 | SER | B2042 | -14.039 | 40.686 | 9.218 | | 40.73 | 0 |
| ATOM | 1222 | N | LEU | B2043 | -14.031 | 38.615 | 8.327 | | 39.91 | N |
| MOTA | 1223 | CA | LEU | B2043 | -12.698 | 38.764 | 7.758 | | 39.34 | C |
| MOTA | 1224 | CB | LEU | B2043 | -11.663 | 38.115 | 8.683 | | 38.78 | c |
| ATOM | 1225 | | | B2043 | -11.484 | 38.654 | 10.105 | | 38.39 | C |
| ATOM | 1226 | CD1 | LEU | B2043 | -10.642 | 37.666 | 10.913 | | 37.70 | С |
| ATOM | 1227 | CD2 | LEU | B2043 | -10.822 | 40.035 | 10.075 | | 37.83 | C |
| MOTA | 1228 | С | LEU | B2043 | -12.555 | 38.165 | 6.360 | | 39.45 | C |
| MOTA | 1229 | | | B2043 | -11.502 | 38.317 | 5.732 | | 39.47 | 0 |
| MOTA | 1230 | | | B2044 | -13.594 | 37.478 | 5.884 | | 38.98 | Ŋ |
| MOTA | 1231 | | | B2044 | -13.569 | 36.850 | 4.556 | | 38.77 | C C |
| MOTA | 1232 | CB | | B2044 | -14.875 | 37.145 | 3.807 | | 39.18 | C |
| MOTA | 1233 | CG | | B2044 | -14.988 | 36.486 | 2.442 | | 38.97 | |
| MOTA | 1234 | CD | | B2044 | -15.072 | 34.973 | 2.556 | | 38.99 | C C |
| ATOM | 1235 | CE | | B2044 | -15.263 | 34.332 | 1.191 | | 38.96 | N |
| MOTA | 1236 | NZ | | B2044 | -15.382 | 32.851 | 1.284 | | 38.96 | C |
| MOTA | 1237 | С | | B2044 | -12.383 | 37.340 | 3.720 | | 38.31 38.14 | 0 |
| MOTA | 1238 | 0 | | B2044 | -12.253 | 38.538 | 3.458 | | 37.92 | N |
| MOTA | 1239 | N | | B2045 | -11.522 | 36.412 | 3.310 | | 36.95 | C |
| ATOM | 1240 | CA | | B2045 | -10.351 | 36.767 | 2.521 | | 36.64 | C |
| ATOM | 1241 | C | | B2045 | -9.108 | 36.124 | 3.108 | | 37.08 | Ö |
| ATOM | 1242 | 0 | | B2045 | -9.207 | 35.141 | 3.845 | | 35.68 | N |
| ATOM | 1243 | N | | B2046 | -7.935 | 36.665 | 2.807 3.332 | | 35.35 | C |
| ATOM | 1244 | CA | | B2046 | -6.703 | 36.084 | 2.750 | | 35.15 | Č |
| ATOM | 1245 | CB | | B2046 | -5.476 | 36.804 | 3.087 | | 35.14 | Ċ |
| ATOM | 1246 | CG | | B2046 | -4.150 | 36.148 34.743 | 2.515 | | 35.11 | č |
| MOTA | 1247 | CD | | B2046 | -4.081 | 34.743 | 2.811 | | 35.11 | N |
| MOTA | 1248 | NE | | B2046 | -2.811 -2.504 | 32.853 | 2.436 | | 35.09 | C |
| ATOM | 1249 | CZ | | B2046 B2046 | -1.323 | 32.338 | 2.748 | | 35.09 | N |
| ATOM | 1250 | | | B2046 | -3.377 | 32.130 | 1.748 | | 35.07 | N. |
| ATOM | 1251 1252 | C | | B2046 | -6.661 | 36.147 | 4.859 | | 34.86 | С |
| ATOM ATOM | 1252 | 0 | | B2046 | -6.273 | 35.184 | 5.522 | • | 34.07 | 0 |
| ATOM | 1254 | N | | B2047 | -7.068 | 37.289 | 5.407 | | 34.76 | N |
| MOTA | 1255 | CA | | B2047 | -7,074 | 37.503 | 6.852 | | 35.00 | C |
| ATOM | 1256 | CB | | B2047 | -7.559 | 38.918 | 7.156 | | 35.75 | С |
| MOTA | 1257 | CG | | B2047 | -6.762 | 39.984 | 6.434 | | 37.57 | С |
| ATOM | 1258 | CD | | B2047 | -7.345 | 41.342 | 6.697 | 1.00 | 39.01 | C |
| ATOM | 1259 | NE | | B2047 | -8.743 | 41.398 | 6.289 | 1.00 | 40.76 | N |
| ATOM | 1260 | CZ | | B2047 | -9.663 | 42.124 | 6.915 | 1.00 | 41.64 | C |
| ATOM | 1261 | | | B2047 | -9.322 | 42.852 | 7.974 | | 41.91 | N |
| ATOM | 1262 | | | B2047 | -10.924 | 42.110 | 6.497 | 1.00 | 42.15 | N |
| ATOM | 1263 | С | | B2047 | -7.959 | 36.483 | 7.566 | 1.00 | 34.24 | C |
| MOTA | 1264 | 0 | ARG | B2047 | -7.681 | 36:070 | 8.692 | | 34.10 | 0 |
| ATOM | 1265 | N | GLN | B2048 | -9.030 | 36.085 | 6.900 | | 33.32 | N |
| ATOM | 1266 | | GLN | B2048 | -9.944 | 35.112 | 7.460 | | 32.27 | С |
| ATOM | 1267 | | GLN | B2048 | -11.138 | 34.961 | 6.531 | | 32.92 | С |
| MOTA | 1268 | | | B2048 | -12.281 | 34.193 | | | 33.21 | C |
| ATOM | 1269 | | | B2048 | -13.323 | 33.871 | 6.077 | | 33.65 | C |
| MOTA | 1270 | | | B2048 | -13.016 | 33.274 | | | 34.07 | 0 |
| MOTA | 1271 | NE2 | | B2048 | -14.567 | 34.258 | | | 33.98 | N |
| MOTA | 1272 | С | | 1 B2048 | -9.224 | 33.772 | | | 31.20 | C |
| MOTA | 1273 | 0 | GL | N B2048 | -9.402 | 33.075 | 8.615 | 1.00 | 30.73 | 0 |

| AROM 1275 CA ILE B2049 -7.661 32.170 6.682 1.00 28.94 C C AROM 1276 CB ILE B2049 -7.007 31.856 5.131 1.00 28.51 C C AROM 1277 CG2 ILE B2049 -6.069 30.658 5.438 1.00 27.59 C C AROM 1278 CG1 ILE B2049 -8.096 31.573 4.267 1.00 28.47 C C AROM 1279 CD1 ILE B2049 -8.096 31.573 4.267 1.00 28.47 C C AROM 1279 CD1 ILE B2049 -6.574 32.195 7.759 1.00 28.73 C C AROM 1280 C ILE B2049 -6.574 32.195 7.759 1.00 28.73 C C AROM 1280 C ILE B2049 -6.574 32.195 7.759 1.00 28.73 C C AROM 1281 O ILE B2049 -6.574 32.195 7.759 1.00 28.34 A AROM 1282 N GU B2050 -5.896 33.336 7.879 1.00 28.34 N AROM 1282 N GU B2050 -4.833 33.494 8.869 1.00 28.07 C C AROM 1285 CG GU B2050 -4.815 34.849 8.665 1.00 29.65 C AROM 1285 CG GU B2050 -2.865 36.279 6.995 1.00 34.62 C AROM 1286 CD GU B2050 -2.865 36.279 6.995 1.00 34.62 C AROM 1289 CD GU B2050 -1.762 36.055 6.430 1.00 35.24 C AROM 1289 CD GU B2050 -4.812 32.768 11.150 1.00 26.78 C AROM 1289 CD GU B2050 -4.812 32.768 11.150 1.00 26.78 C AROM 1290 O GU B2050 -4.812 32.768 11.150 1.00 26.09 N AROM 1291 N TWR B2051 -6.600 33.944 10.453 1.00 25.41 N AROM 1292 CA TWR B2051 -7.251 33.868 11.749 1.00 24.34 C AROM 1293 CB TWR B2051 -8.535 34.703 11.741 1.00 23.37 C AROM 1295 CD TWR B2051 -8.535 34.703 11.741 1.00 23.37 C AROM 1295 CD TWR B2051 -9.316 33.559 14.039 1.00 22.86 C C AROM 1295 CD TWR B2051 -9.316 33.559 14.059 1.00 22.86 C C AROM 1295 CD TWR B2051 -9.657 35.284 15.332 1.00 22.31 C C AROM 1300 O TWR B2051 -10.347 33.695 13.169 1.00 22.86 C C TWR B2051 -9.657 35.284 15.332 1.00 22.31 C C AROM 1300 O TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C AROM 1300 O TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C AROM 1300 O TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C AROM 1300 O TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.169 1.00 22.91 C C TWR B2051 -10.437 33.695 13.190 13.154 1.00 22.9 | | | | | 50040 | 0.40 | E 2 | 2 410 | 6.634 | 1 00 | 29 96 | N |
|--|------|------|-----|------|---------|-------|------|--------|--------|------|-------|---|
| ATOM 1276 CB ILE B2049 | MOTA | 1274 | | | | | | | | | | |
| ATOM 1278 CG2 ILE 22049 | | | | | | | | | | | | |
| ATOM 1279 CG1 ILE 82049 -8.096 31.573 4.267 1.00 28.47 ATOM 1280 C ILE 82049 -8.950 30.333 4.553 1.00 27.80 C ATOM 1281 O ILE 82049 -6.574 32.198 7.759 1.00 28.73 C ATOM 1281 O ILE 82049 -6.574 32.198 7.759 1.00 28.73 C ATOM 1282 N GU 82050 -5.896 33.336 7.879 1.00 28.38 N ATOM 1283 CA GLU 82050 -4.833 33.494 8.859 1.00 28.07 C ATOM 1283 CA GLU 82050 -4.833 33.494 8.859 1.00 29.65 C ATOM 1285 CG GLU 82050 -4.813 34.848 8.665 1.00 29.65 C ATOM 1285 CG GLU 82050 -3.799 35.103 7.200 1.00 34.62 C ATOM 1287 OEI GLU 82050 -3.232 37.416 7.392 1.00 35.24 O ATOM 1287 OEI GLU 82050 -1.762 36.055 6.430 1.00 35.19 O ATOM 1289 C GLU 82050 -5.416 33.374 10.260 1.00 26.78 ATOM 1289 C GLU 82050 -4.812 32.768 11.150 1.00 26.09 ATOM 1289 C GLU 82050 -4.812 32.768 11.150 1.00 26.09 N ATOM 1291 N TYR 82051 -6.600 33.944 10.453 1.00 25.41 N ATOM 1292 CA TYR 82051 -7.251 33.868 11.744 1.00 23.37 C ATOM 1293 CB TYR 82051 -9.316 34.703 11.741 1.00 23.37 C ATOM 1295 CD TYR 82051 -9.316 34.618 13.024 1.00 22.77 ATOM 1295 CD TYR 82051 -9.316 34.618 13.024 1.00 22.77 C ATOM 1295 CD TYR 82051 -9.316 34.618 13.024 1.00 22.77 C ATOM 1295 CD TYR 82051 -9.316 34.618 13.024 1.00 22.77 C ATOM 1295 CD TYR 82051 -9.316 34.618 13.024 1.00 22.77 C ATOM 1295 CD TYR 82051 -9.573 32.400 12.086 1.00 23.14 C ATOM 1295 CD TYR 82051 -9.573 32.400 12.086 1.00 23.14 C ATOM 1301 C TYR 82051 -10.037 34.350 15.450 1.00 23.43 C ATOM 1301 C TYR 82051 -7.750 32.400 12.086 1.00 23.43 A ATOM 1301 C TYR 82051 -7.750 32.400 12.086 1.00 23.43 A ATOM 1301 C TYR 82051 -9.577 35.284 15.332 1.00 23.14 C ATOM 1303 N LEU 82052 -8.541 30.291 11.364 1.00 22.95 ATOM 1303 N LEU 82052 -9.598 28.247 10.086 1.00 22.55 ATOM 1306 CB LEU 82052 -7.242 29.748 10.133 1.00 22.55 ATOM 1307 CD LEU 82052 -7.242 29.748 10.133 1.00 22.55 ATOM 1308 CD LEU 82052 -7.244 29.757 11.622 1.00 22.55 ATOM 1307 CD LEU 82052 -7.242 29.748 10.133 1.00 22.55 ATOM 1310 O LEU 82052 -7.242 29.748 10.133 1.00 22.55 ATOM 1311 O ALA B2053 -7.4072 29.322 99.774 1.00 22.35 ATOM 1312 CA ALA B2053 -7.406 29.91 30.88 | MOTA | | | | | | | | | | | |
| ATOM 1279 CD1 ILE 82049 | ATOM | | | | | | | | | | | |
| ATOM 1280 C ILE 22049 | MOTA | 1278 | CG1 | ILE | B2049 | | | | | | | |
| ATOM 1281 O ILE B2049 | MOTA | 1279 | | | | | | | | | | |
| ATOM 1282 N GLU B2050 | MOTA | 1280 | С | ILE | B2049 | | | | | | | |
| ATOM 1283 CA GIU B2050 | ATOM | 1281 | 0 | ILE | B2049 | | | | | | | |
| ATOM 1284 CB GJU B2050 | MOTA | 1282 | N | GLU | B2050 | -5.89 | 96 3 | 3.336 | | | | |
| ATOM 1285 CG GLU B2050 -3.799 35.103 7.200 1.00 32.92 C ATOM 1286 CD GLU B2050 -3.292 37.416 7.392 1.00 34.62 C ATOM 1287 OB1 GLU B2050 -3.232 37.416 7.392 1.00 35.24 O ATOM 1288 OB2 GLU B2050 -1.762 36.055 6.430 1.00 35.19 O ATOM 1289 C GLU B2050 -5.416 33.374 10.260 1.00 26.78 C ATOM 1290 O GLU B2050 -4.812 32.768 11.150 1.00 26.09 ATOM 1291 N TYR B2051 -6.600 33.944 10.453 1.00 25.41 N ATOM 1292 CA TYR B2051 -7.551 33.868 11.741 1.00 24.34 C ATOM 1293 CB TYR B2051 -9.516 34.618 13.024 1.00 22.77 ATOM 1293 CG TYR B2051 -9.516 34.618 13.024 1.00 22.77 C ATOM 1295 CD TYR B2051 -10.347 33.695 13.169 1.00 22.86 ATOM 1296 CE1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 ATOM 1296 CE1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 C ATOM 1296 CE2 TYR B2051 -8.984 35.413 14.116 1.00 22.81 ATOM 1298 CE2 TYR B2051 -9.657 35.284 15.332 1.00 23.14 ATOM 1299 CZ TYR B2051 -10.077 34.350 15.450 1.00 23.03 ATOM 1300 OH TYR B2051 -11.322 34.186 16.649 1.00 23.03 ATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 24.05 ATOM 1301 C TYR B2051 -7.150 32.400 12.086 1.00 24.05 ATOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 ATOM 1304 CA EUB 22052 -8.211 31.700 11.170 1.00 23.25 ATOM 1305 CB LEU B2052 -8.211 31.700 11.170 1.00 23.25 ATOM 1306 CG LEU B2052 -9.274 29.748 10.133 1.00 22.91 ATOM 1307 CDL EUB 22052 -9.274 29.748 10.133 1.00 22.91 ATOM 1308 CDZ LEU B2052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1309 C LEU B2052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1309 C LEU B2052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1307 CDL EUB 22052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1307 CDL EUB 22052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1309 C LEU B2052 -7.224 29.748 10.133 1.00 22.95 CA ATOM 1310 C ALA B2053 -6.265 39.96 12.57 11.00 22.91 CA ATOM 1311 N ALA B2053 -6.265 39.96 12.57 11.00 22.91 CA ATOM 1312 CA ALA B2053 -6.266 31.042 11.500 21.95 CA ATOM 1312 CA ALA B2053 -6.266 31.042 11.500 21.195 CA ATOM 1313 CA ALA B2053 -6.266 31.042 11.00 21.195 CA ATOM 1312 CA ALA B2053 -6.266 31.046 1.00 22.13 1.00 21.195 CA ATOM 1322 CB ARG B2055 | ATOM | 1283 | CA | GLU | B2050 | -4.83 | | | | | | |
| ATOM 1285 CG GLU B2050 -3.799 35.103 7.200 1.00 32.92 CG ATOM 1286 CD GLU B2050 -2.865 36.279 6.995 1.00 34.62 CC ATOM 1287 OE1 GLU B2050 -3.232 37.416 7.392 1.00 35.24 OTOM 1288 OE2 GLU B2050 -1.762 36.055 6.430 1.00 35.19 OTOM 1289 C GLU B2050 -5.416 33.374 10.260 1.00 26.78 CTOM 1290 C GLU B2050 -4.812 32.768 11.150 1.00 26.78 CTOM 1291 N TYR B2051 -6.600 33.944 10.453 1.00 25.41 NT ATOM 1292 CA TYR B2051 -7.251 33.868 11.749 1.00 24.34 ATOM 1293 CB TYR B2051 -9.316 34.618 13.024 1.00 22.77 CTOM 1294 CG TYR B2051 -9.916 34.618 13.024 1.00 22.77 CTOM 1295 CD1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 CTOM 1296 CE1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 CTOM 1297 CD2 TYR B2051 -9.657 34.350 15.450 1.00 22.81 CTOM 1298 CE2 TYR B2051 -9.657 35.284 15.332 1.00 23.14 CTOM 1299 CZ TYR B2051 -10.677 34.350 15.450 1.00 23.43 CTOM 1290 CT TYR B2051 -11.332 34.186 16.649 1.00 23.43 CTOM 1300 OH TYR B2051 -11.332 34.186 16.649 1.00 23.43 CTOM 1301 C TYR B2051 -7.176 31.910 13.154 1.00 24.05 CTOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 CTOM 1304 CA LEU B2052 -8.211 31.700 11.170 1.00 22.85 CTOM 1305 CB LEU B2052 -9.274 29.748 10.133 1.00 22.55 CTOM 1306 CG LEU B2052 -9.274 29.748 10.133 1.00 22.85 CTOM 1307 CD1 LEU B2052 -7.224 29.748 10.133 1.00 22.91 CTOM 1308 CD2 LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1309 C LEU B2052 -7.224 29.748 10.133 1.00 22.95 CTOM 1301 C CTOM B2052 -7.224 29.748 10.133 1.00 22.95 CTOM 1302 CALB B2053 -4.072 29.748 10.133 1.00 22.95 CTOM 1303 N LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1304 CA LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1305 CB LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1306 CG LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1307 CD1 LEU B2052 -9.274 29.748 10.133 1.00 22.95 CTOM 1308 CD2 LEU B2052 -9.284 29.748 10.133 1.00 22.95 CTOM 1309 C LEU B2052 -9.286 28.295 10.368 1.00 22.19 CTOM 1310 N AGR B2053 -6.668 1.00 244 1.00 22.13 CTOM 1311 N ALA B2053 -6.265 30.468 1.00 24.405 CTOM 1320 N ARG B2055 -6.626 34.473 16.832 1.00 20.08 CTOM 1322 C ARG | | 1284 | CB | GLU | B2050 | -4.15 | 51 3 | 4.848 | | | | |
| ATOM 1286 CD GLU B2050 | | | CG | GLU | B2050 | -3.79 | 99 3 | 5.103 | | | | |
| ATOM 1288 OE2 GLU B2050 | | | CD | GLU | B2050 | -2.8 | 55 3 | 6.279 | | | | |
| ATOM 1288 OE2 GLU B2050 -1.762 36.055 6.430 1.00 35.19 C ATOM 1289 C GLU B2050 -5.416 33.374 10.260 1.00 26.78 C ATOM 1291 N TYR B2051 -6.600 33.944 10.453 1.00 25.41 N ATOM 1292 CA TYR B2051 -7.251 33.868 11.749 1.00 24.34 C ATOM 1293 CB TYR B2051 -8.535 34.703 11.741 1.00 24.34 C ATOM 1295 CD1 TYR B2051 -9.316 34.618 13.024 1.00 22.77 C ATOM 1295 CD1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 C ATOM 1295 CD1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 C ATOM 1296 CE1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 C ATOM 1296 CE2 TYR B2051 -8.984 35.413 14.116 1.00 22.81 ATOM 1298 CE2 TYR B2051 -9.657 35.284 15.332 1.00 23.14 ATOM 1298 CE2 TYR B2051 -10.677 34.350 15.450 10.00 23.03 ATOM 1300 OH TYR B2051 -11.322 34.186 16.649 1.00 23.03 ATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 23.03 ATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 24.55 ATOM 1302 O TYR B2051 -7.176 31.910 13.154 1.00 24.55 ATOM 1305 CB LEU B2052 -8.511 31.700 11.170 1.00 23.25 NATOM 1305 CB LEU B2052 -8.541 30.291 11.364 1.00 22.91 ATOM 1306 CG LEU B2052 -9.598 28.247 10.086 1.00 22.55 ATOM 1307 CD1 LEU B2052 -9.598 28.247 10.086 1.00 22.55 ATOM 1308 CD2 LEU B2052 -9.598 28.247 10.086 1.00 22.55 ATOM 1301 C LEU B2052 -7.284 29.457 11.622 1.00 22.689 ATOM 1301 N ALA B2053 -6.285 29.612 10.761 1.00 22.31 ATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.31 ATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.31 ATOM 1311 C ALA B2053 -4.072 29.332 9.774 1.00 21.95 ATOM 1311 C ALA B2053 -4.072 29.332 9.774 1.00 21.95 ATOM 1311 C ALA B2053 -4.072 29.332 9.774 1.00 21.95 ATOM 1311 C ALA B2053 -6.285 29.612 10.761 1.00 22.91 ATOM 1312 C A ALA B2053 -6.285 29.612 10.761 1.00 22.31 ATOM 1312 C A ALA B2053 -6.285 29.612 10.761 1.00 22.91 ATOM 1312 C A ALA B2053 -6.285 29.612 10.761 1.00 22.91 ATOM 1312 C A ALA B2053 -6.285 29.612 10.761 1.00 21.95 ATOM 1322 C B ARG B2055 -8.685 30.0427 12.688 1.00 21.95 ATOM 1322 C B ARG B2055 -6.681 29.290 16.114 1.00 20.99 ATOM 1322 C B ARG B2055 -7.664 34.473 16.832 1.00 20.73 ATOM 1322 C B ARG B2055 -7.664 34.473 1 | | | OE1 | GLU | B2050 | -3.2 | 32 3 | 7.416 | 7.392 | | | |
| ATOM 1289 C GLU B2050 | | | | | | -1.7 | 52 3 | 6.055 | 6.430 | | | |
| ATOM 1290 O GLU B2050 -4.812 32.768 11.150 1.00 26.09 O ATOM 1291 N TYR B2051 -6.600 33.944 10.453 1.00 25.41 N ATOM 1292 CA TYR B2051 -7.251 33.868 11.749 1.00 24.34 C ATOM 1292 CB TYR B2051 -8.535 34.703 11.741 1.00 23.37 C ATOM 1294 CG TYR B2051 -9.535 34.703 11.741 1.00 22.37 C ATOM 1295 CD1 TYR B2051 -9.316 34.618 13.024 1.00 22.77 ATOM 1295 CD1 TYR B2051 -10.347 33.695 13.169 1.00 22.86 C ATOM 1297 CD2 TYR B2051 -8.884 35.413 14.116 1.00 22.81 ATOM 1297 CD2 TYR B2051 -9.657 35.284 15.332 1.00 23.14 C ATOM 1299 CZ TYR B2051 -9.657 35.284 15.332 1.00 23.14 C ATOM 1299 CZ TYR B2051 -10.677 34.350 15.450 1.00 23.43 ATOM 1300 OH TYR B2051 -7.550 32.400 12.086 1.00 24.05 ATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 24.05 ATOM 1302 O TYR B2051 -7.176 31.910 31.514 1.00 24.52 ATOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 ATOM 1304 CA LEU B2052 -8.211 31.700 11.170 1.00 23.25 ATOM 1305 CB LEU B2052 -9.274 29.746 10.133 1.00 22.95 ATOM 1306 CG LEU B2052 -9.598 28.247 10.086 1.00 22.95 ATOM 1308 CD2 LEU B2052 -9.598 28.247 10.086 1.00 22.95 ATOM 1309 C LEU B2052 -7.284 29.745 10.133 1.00 22.95 ATOM 1309 C LEU B2052 -7.284 29.745 10.086 1.00 22.95 ATOM 1301 C ALB B2053 -6.285 29.612 10.761 1.00 22.99 ATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.94 ATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.94 ATOM 1313 C A ALA B2053 -6.285 29.612 10.761 1.00 22.94 ATOM 1316 N GLY B2054 -3.986 29.678 16.049 1.00 21.35 ATOM 1316 N GLY B2054 -3.985 29.612 10.761 1.00 21.35 ATOM 1316 N GLY B2054 -3.986 29.678 16.049 1.00 21.95 ATOM 1312 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1316 N GLY B2054 -3.986 29.678 16.049 1.00 21.95 ATOM 1312 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1316 N GLY B2054 -3.986 29.678 16.049 1.00 21.95 ATOM 1312 CA ARG B2055 -8.594 29.976 16.040 1.00 21.35 ATOM 1312 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1312 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -6.661 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -6.662 33.046 17.669 1.00 20.73 AT | | | | | | -5.4 | 16 3 | 3.374 | 10.260 | | | |
| ATOM 1291 N TYR B2051 | | | | | | -4.8 | 12 3 | 2.768 | 11.150 | | | |
| ATOM 1292 CA TYR B2051 | | | | | | -6.6 | 00 3 | 3.944 | 10.453 | 1.00 | 25.41 | |
| ATOM 1293 CB TYR B2051 | | | | | | • | | 3.868 | 11.749 | 1.00 | 24.34 | |
| ATOM 1294 CG TYR B2051 | | | | | | | | | 11.741 | 1.00 | 23.37 | |
| ATOM 1295 CD1 TYR B2051 | | | | | | | | | 13.024 | 1.00 | 22.77 | |
| ATOM 1296 CE1 TYR B2051 -11.026 33.559 14.369 1.00 23.29 CATOM 1297 CD2 TYR B2051 -8.984 35.413 14.116 1.00 22.81 CATOM 1299 CZ TYR B2051 -9.657 35.284 15.332 1.00 23.14 CATOM 1299 CZ TYR B2051 -10.677 34.350 15.450 1.00 23.34 CATOM 1300 OH TYR B2051 -11.332 34.186 16.649 1.00 23.03 OATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 24.05 CATOM 1302 O TYR B2051 -7.176 31.910 13.154 1.00 24.52 OATOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 NATOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 NATOM 1305 CB LEU B2052 -9.274 29.748 10.133 1.00 22.91 CATOM 1306 CG LEU B2052 -9.598 28.247 10.086 1.00 22.85 CATOM 1307 CD1 LEU B2052 -10.345 27.814 11.343 1.00 21.95 CATOM 1308 CD2 LEU B2052 -10.436 27.957 8.835 1.00 22.89 CATOM 1310 O LEU B2052 -7.234 29.457 11.622 1.00 22.68 CATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.91 CATOM 1312 CA ALA B2053 -5.024 28.897 10.884 12.571 1.00 22.94 CATOM 1313 CB ALA B2053 -5.024 28.897 10.884 1.00 21.99 CATOM 1315 OALA B2053 -4.397 29.180 12.244 1.00 22.13 ATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.99 CATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1317 CA GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1317 CA GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1317 CA GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 CATOM 1320 N ARG B2055 -5.974 29.976 15.040 1.00 20.89 CATOM 1321 CA ALA B2053 -4.592 29.512 10.761 1.00 22.13 CATOM 1321 CA ALA B2053 -4.592 29.612 10.761 1.00 22.13 CATOM 1322 CA ARG B2055 -6.681 29.691 10.761 1.00 20.89 CATOM 1322 CA ARG B2055 -6.681 29.691 10.761 10.00 20.89 CATOM 1322 CA ARG B2055 -6.681 29.691 10.761 10.00 20.89 CATOM 1322 CA ARG B2055 -7.264 13.986 16.664 1.00 20.09 10.00 20.73 CATOM 1322 CA ARG B2055 -7.634 34.216 17.668 1.00 20.07 10.00 20.73 CATOM 1322 CA ARG B2055 -7.634 34.216 17.668 1.00 20.07 10.00 | | | | | | | | | 13.169 | 1.00 | 22.86 | С |
| ATOM 1297 CD2 TYR B2051 | | | | | | | | | 14.369 | 1.00 | 23.29 | С |
| ATOM 1298 CE2 TYR B2051 | | | | | | | | | | | | C |
| ATOM 1299 CZ TYR B2051 -10.677 34.350 15.450 1.00 23.43 CATOM 1300 OH TYR B2051 -11.332 34.186 16.649 1.00 23.03 OATOM 1301 C TYR B2051 -7.550 32.400 12.086 1.00 24.05 CATOM 1303 N LEU B2052 -8.211 31.700 11.170 1.00 23.25 NATOM 1303 N LEU B2052 -8.541 30.291 11.364 1.00 22.55 CATOM 1306 CB LEU B2052 -9.274 29.748 10.133 1.00 22.55 CATOM 1306 CG LEU B2052 -9.598 28.247 10.086 1.00 22.85 CATOM 1308 CD2 LEU B2052 -10.436 27.814 11.343 1.00 22.85 CATOM 1309 C LEU B2052 -10.436 27.957 8.835 1.00 22.89 CATOM 1300 C LEU B2052 -7.284 29.457 11.622 1.00 22.68 CATOM 1310 O LEU B2052 -7.284 29.457 11.622 1.00 22.68 CATOM 1311 N ALA B2053 -6.285 29.612 10.761 1.00 22.31 NATOM 1313 CB ALA B2053 -4.372 29.332 9.774 1.00 21.32 ATOM 1314 C ALA B2053 -4.072 29.332 9.774 1.00 21.32 ATOM 1316 N GLY B2054 -4.532 30.427 12.668 1.00 21.87 ATOM 1316 N GLY B2054 -4.532 30.427 12.668 1.00 21.87 ATOM 1317 CA GLY B2054 -4.532 30.427 12.668 1.00 21.95 ATOM 1318 C GLY B2054 -3.981 30.829 13.963 1.00 21.95 ATOM 1319 O GLY B2054 -4.532 30.427 12.668 1.00 21.87 ATOM 1319 O GLY B2054 -4.532 30.427 12.668 1.00 21.87 ATOM 1318 C GLY B2054 -3.981 30.829 13.963 1.00 21.95 ATOM 1319 O GLY B2054 -4.654 30.111 15.107 1.00 21.35 ATOM 1312 CA ARG B2055 -5.974 29.976 15.040 1.00 22.13 ATOM 1312 CA ARG B2055 -5.974 29.976 15.040 1.00 20.89 ATOM 1320 N ARG B2055 -5.994 29.976 15.040 1.00 20.89 ATOM 1322 CB ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.685 30.688 16.934 1.00 19.79 ATOM 1322 CB ARG B2055 -8.685 30.688 16.934 1.00 19.79 ATOM 1325 NE ARG B2055 -8.685 30.688 16.934 1.00 20.08 ATOM 1325 NE ARG B2055 -6.626 34.473 16.832 1.00 20.13 ATOM 1326 CZ ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1328 NH2 ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1328 NH2 ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1328 NH2 ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1328 NH2 ARG B2055 -6.626 34.473 16.832 1.00 20.91 ATOM 1328 NH2 ARG B2055 -6.626 34.473 16.832 1.00 20.93 | | | | | | | _ | | | | | С |
| ATOM 1299 CZ 11R 82051 -11.332 34.186 16.649 1.00 23.03 ATOM 1301 C TYR 82051 -7.550 32.400 12.086 1.00 24.05 CC ATOM 1302 O TYR 82051 -7.176 31.910 13.154 1.00 24.52 NC ATOM 1303 N LEU 82052 -8.211 31.700 11.170 1.00 23.25 NC ATOM 1304 CA LEU 82052 -8.541 30.291 11.364 1.00 22.91 ATOM 1305 CB LEU 82052 -9.274 29.748 10.133 1.00 22.55 ATOM 1306 CG LEU 82052 -9.598 28.247 10.086 1.00 22.85 ATOM 1307 CD1 LEU 82052 -9.598 28.247 10.086 1.00 22.85 ATOM 1308 CD2 LEU 82052 -10.345 27.814 11.343 1.00 21.95 ATOM 1309 C LEU 82052 -7.234 29.457 11.622 1.00 22.68 ATOM 1310 O LEU 82052 -7.232 28.681 12.571 1.00 22.94 ATOM 1311 N ALA 82053 -6.285 29.612 10.761 1.00 22.31 NATOM 1312 CA ALA 82053 -5.024 28.897 10.884 1.00 21.99 ATOM 1313 CB ALA 82053 -4.072 29.332 9.774 1.00 21.32 ATOM 1315 O ALA 82053 -4.072 29.332 9.774 1.00 22.13 ATOM 1315 O ALA 82053 -4.072 29.332 9.74 1.00 22.13 ATOM 1316 N GLY 82054 -4.532 30.427 12.688 1.00 21.87 ATOM 1317 CA GLY 82054 -4.532 30.427 12.688 1.00 21.87 ATOM 1318 C GLY 82054 -4.654 30.111 15.107 1.00 21.35 ATOM 1319 O GLY 82054 -4.654 30.111 15.107 1.00 21.35 ATOM 1319 O GLY 82054 -4.654 30.111 15.107 1.00 21.35 ATOM 1312 CA ARG 82055 -5.974 29.976 15.040 1.00 20.89 ATOM 1322 CB ARG 82055 -8.191 29.543 16.034 1.00 20.89 ATOM 1322 CB ARG 82055 -8.685 33.046 17.609 1.00 20.89 ATOM 1322 CB ARG 82055 -8.685 33.046 17.609 1.00 20.08 ATOM 1322 CB ARG 82055 -8.665 33.046 17.609 1.00 20.08 ATOM 1325 NE ARG 82055 -8.665 33.046 17.609 1.00 20.08 ATOM 1325 NE ARG 82055 -8.665 33.046 17.609 1.00 20.91 ATOM 1326 CZ ARG 82055 -8.665 33.046 17.609 1.00 20.91 ATOM 1326 CZ ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1326 CZ ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1326 CZ ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL ARG 82055 -6.626 34.473 16.832 1.00 20.13 ATOM 1328 NL | | | | | | | | | | | | C |
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| ATOM 1314 C ALA B2053 | MOTA | | | | | | | | | | | Ċ |
| ATOM 1314 C ALA B2053 | | | | | | | | | | | | Č |
| ATOM 1316 N GLY B2054 -4.532 30.427 12.688 1.00 21.95 ATOM 1317 CA GLY B2054 -3.981 30.829 13.963 1.00 21.46 ATOM 1318 C GLY B2054 -4.654 30.111 15.107 1.00 21.35 ATOM 1319 O GLY B2054 -3.986 29.678 16.049 1.00 21.19 ATOM 1320 N ARG B2055 -5.974 29.976 15.040 1.00 20.89 ATOM 1321 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1323 CG ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | ATOM | | С | | | | | | | | | Ö |
| ATOM 1316 N GBI B2054 -3.981 30.829 13.963 1.00 21.46 ATOM 1318 C GLY B2054 -4.654 30.111 15.107 1.00 21.35 ATOM 1319 O GLY B2054 -3.986 29.678 16.049 1.00 21.19 ATOM 1320 N ARG B2055 -5.974 29.976 15.040 1.00 20.89 ATOM 1321 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1323 CG ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | ATOM | 1315 | 0 | | | | | | | | | N |
| ATOM 1318 C GLY B2054 -4.654 30.111 15.107 1.00 21.35 ATOM 1319 O GLY B2054 -3.986 29.678 16.049 1.00 21.19 ATOM 1320 N ARG B2055 -5.974 29.976 15.040 1.00 20.89 ATOM 1321 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1323 CG ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | ATOM | | | | | | | | | | | C |
| ATOM 1318 C GLY B2054 ATOM 1319 O GLY B2054 ATOM 1320 N ARG B2055 ATOM 1321 CA ARG B2055 ATOM 1322 CB ARG B2055 ATOM 1323 CG ARG B2055 ATOM 1324 CD ARG B2055 ATOM 1325 NE ARG B2055 ATOM 1325 NE ARG B2055 ATOM 1326 CZ ARG B2055 ATOM 1327 NH1 ARG B2055 ATOM 1328 NH2 ARG B2055 ATOM 1328 NH2 ARG B2055 ATOM 1329 C ARG B2055 ATOM 1329 C ARG B2055 ATOM 1329 C ARG B2055 ATOM 1328 NH2 ARG B2055 ATOM 1329 C ARG B2055 | ATOM | 1317 | CA | | | | | | | | | C |
| ATOM 1320 N ARG B2055 -5.974 29.976 15.040 1.00 20.89 ATOM 1321 CA ARG B2055 -6.681 29.290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1323 CG ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1318 | С | | | | | | | | | 0 |
| ATOM 1321 CA ARG B2055 -6.681 29:290 16.114 1.00 20.89 ATOM 1322 CB ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1323 CG ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1319 | 0 | | | | | | | | | N |
| ATOM 1321 CA ARG B2055 -8.191 29.543 16.034 1.00 20.27 ATOM 1322 CB ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1320 | N | | | | | | | | | C |
| ATOM 1322 CB ARG B2055 -8.685 30.688 16.934 1.00 19.89 ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1321 | CA | | | | | | | | | C |
| ATOM 1324 CD ARG B2055 -7.926 31.986 16.664 1.00 20.08 ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1322 | CB | | | | | | | | | C |
| ATOM 1324 CD ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1325 NE ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | MOTA | 1323 | CG | | | | | | | | | |
| ATOM 1325 NE ARG B2055 -8.265 33.046 17.609 1.00 19.79 ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | | 1324 | CD | | | | | | | | | C |
| ATOM 1326 CZ ARG B2055 -7.634 34.216 17.668 1.00 20.91 ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | | | | ARG | G B2055 | | | | | | | N |
| ATOM 1327 NH1 ARG B2055 -6.626 34.473 16.832 1.00 20.64 ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | | | | ARG | G B2055 | | | | | | | C |
| ATOM 1328 NH2 ARG B2055 -8.009 35.135 18.555 1.00 20.13 ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | | 1327 | | | | | | | | | | N |
| ATOM 1329 C ARG B2055 -6.383 27.796 16.086 1.00 20.73 | | 1328 | NH2 | 2 AR | G B2055 | -8. | 009 | | | | | И |
| | | | | AR | G B2055 | | | | | | | C |
| | MOTA | | | AR | G B2055 | -6. | 239 | 27.169 | 17.136 | 1.0 | 20.29 | 0 |

| MOTA | 1331 | N | TRP | B2056 | -6:273 | 27.235 | 14.884 | 1.00 20.69 | N |
|--------------|--------------|----------|-----|----------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 1332 | CA | TRP | B2056 | -5.976 | 25.817 | 14.742 | 1.00 20.72 | C |
| ATOM | 1333 | CB | TRP | B2056 | -5.992 | 25.408 | 13.262 | 1.00 21.90 | С |
| ATOM | 1334 | CG | TRP | B2056 | -5.402 | 24.051 | 13.020 | 1.00 23.77 | С |
| ATOM | 1335 | CD2 | TRP | B2056 | -6.116 | 22.814 | 12.903 | 1.00 24.30 | · C |
| MOTA | 1336 | CE2 | TRP | B2056 | -5.151 | 21.780 | 12.814 | 1.00 24.91 | C |
| ATOM | 1337 | CE3 | TRP | B2056 | -7.473 | 22.478 | 12.869 | 1.00 24.91 | С |
| ATOM | 1338 | CD1 | TRP | B2056 | -4.065 | 23.727 | 12.983 | 1.00 23.97 | С |
| MOTA | 1339 | NE1 | TRP | B2056 | -3.912 | 22.365 | 12.864 | 1.00 24.86 | N |
| MOTA | 1340 | CZ2 | TRP | B2056 | -5.50 5 | 20.429 | 12.697 | 1.00 25.50 | С |
| ATOM | 1341 | CZ3 | TRP | B2056 | -7.829 | 21.131 | 12.751 | 1.00 26.26 | С |
| ATOM | 1342 | CH2 | TRP | B2056 | -6.843 | 20.122 | 12.667 | 1.00 26.22 | С |
| MOTA | 1343 | С | TRP | B2056 | -4.603 | 25.547 | 15.348 | 1.00 20.41 | С |
| ATOM | 1344 | 0 | TRP | B2056 | -4.409 | 24.582 | 16.093 | 1.00 20.04 | 0 |
| ATOM | 1345 | N | | B2057 | -3.654 | 26.415 | 15.025 | 1.00 19.64 | N |
| ATOM | 1346 | CA | | B2057 | -2.298 | 26.282 | 15.533 | 1.00 19.83 | C |
| ATOM | 1347 | CB | - | B2057 | -1.395 | 27.339 | 14.898 | 1.00 20.26 | C |
| MOTA | 1348 | OG | | B2057 | -0.057 | 27.136 | 15.303 | 1.00 22.97 | 0 |
| ATOM | 1349 | С | | B2057 | -2.239 | 26.402 | 17.062 | 1.00 18.86 | C |
| ATOM | 1350 | 0 | | B2057 | -1.548 | 25.636 | 17.725 | 1.00 18.27 | 0 |
| MOTA | 1351 | N | | B2058 | -2.968 | 27.367 | 17.613 | 1.00 18.16 | N |
| ATOM | 1352 | CA | | B2058 | -2.996 | 27.566 | 19.058 | 1.00 17.01 | C |
| ATOM | 1353 | CB | | B2058 | -3.767 | 28.826 | 19.388 | 1.00 16.89 | C |
| ATOM | 1354 | C | | B2058 | -3.623 | 26.365 | 19.781 20.783 | 1.00 16.76 | C 0 |
| ATOM | 1355 1356 | O N | | B2058 | -3.087 -4.755 | 25.890 | 19.272 | 1.00 15.81 1.00 16.40 | Ŋ |
| ATOM | 1357 | N Ch | | B2059 B2059 | -5.446 | 25.884 24.746 | 19.883 | 1.00 17.29 | C |
| ATOM ATOM | 1358 | CA CB | | B2059 | -6.815 | 24.740 | 19.003 | 1.00 17.23 | c |
| ATOM | 1359 | CG | | B2059 | -7.751 | 25.730 | 19.498 | 1.00 15.32 | c |
| ATOM | 1360 | CD | | B2059 | -9.168 | 25.536 | 18.996 | 1.00 14.90 | C |
| ATOM | 1361 | CE | | B2059 | -10.011 | 26.783 | 19.319 | 1.00 13.82 | č |
| ATOM | 1362 | NZ | | B2059 | -11.432 | 26.637 | 18.937 | 1.00 11.65 | N |
| ATOM | 1363 | C | | B2059 | -4.620 | 23.464 | 19.826 | 1.00 17.91 | C |
| ATOM | 1364 | 0 | | B2059 | -4.640 | 22.656 | 20.748 | 1.00 16.96 | 0 |
| ATOM | 1365 | N | | B2060 | -3.879 | 23.293 | 18.738 | 1.00 19.43 | N |
| MOTA | 1366 | CA | | B2060 | -3.043 | 22.123 | 18.585 | 1.00 20.86 | С |
| ATOM | 1367 | CB | GLU | B2060 | -2.516 | 22.046 | 17.146 | 1.00 22.77 | С |
| MOTA | 1368 | CG | GLU | B2060 | -1.964 | 20.691 | 16.759 | 1.00 26.37 | С |
| MOTA | 1369 | CD | GLU | B2060 | -2.982 | 19.574 | 16.959 | 1.00 29.21 | C |
| MOTA | 1370 | OE1 | GLU | B2060 | -4.047 | 19.602 | 16.287 | 1.00 29.92 | 0 |
| ATOM | 1371 | OE2 | GLU | B2060 | -2.720 | 18.670 | 17.795 | 1.00 30.31 | 0 |
| MOTA | 1372 | С | | B2060 | -1.889 | 22.256 | 19.593 | 1.00 20.86 | С |
| MOTA | 1373 | 0 | | B2060 | -1.556 | 21.302 | 20.307 | 1.00 20.96 | 0 |
| MOTA | 1374 | N | | B2061 | -1.299 | 23.447 | 19.661 | 1.00 20.25 | N |
| ATOM | 1375 | CA | | B2061 | -0.191 | 23.697 | 20.580 | 1.00 20.38 | С |
| MOTA | 1376 | CB | | B2061 | | | | 1.00 19.50 | C |
| ATOM | 1377 | C | | B2061 | -0.655 | 23.464 | 22.015 | 1.00 20.28 | C |
| MOTA | 1378 | 0 | | B2061 B2062 | 0.103 | 22:952 23.832 | 22.841 | 1.00 20.05 1.00 20.49 | О N |
| ATOM | 1379 | N CT | | | -1.896 | | 22.313 | | C |
| MOTA MOTA | 1380 1381 | CA CB | | B2062 B2062 | -2.419 -3.738 | 23.620 24.382 | 23.659 23.880 | 1.00 21.41 | C |
| ATOM | 1382 | CG | | B2062 | -4.350 | 24.362 | 25.242 | 1.00 21.20 | C |
| ATOM | 1383 | | | B2062 | -5.134 | 23.015 | 25.481 | 1.00 21.03 | č |
| ATOM | 1384 | | | B2062 | -4.092 | 25.019 | 26.297 | 1.00 21.77 | Č |
| ATOM | 1385 | | | B2062 | -5.646 | 22.756 | 26.745 | 1.00 21.47 | č |
| ATOM | 1386 | | | B2062 | -4.603 | 24.757 | 27.576 | 1.00 22.09 | c |
| ATOM | 1387 | CZ | | B2062 | -5.382 | 23.627 | 27.799 | 1.00 21.52 | С |
| | | | | | | | | | |

| MOTA | 1388 | С | PHE | B2062 | -2.630 | 22.133 | 23.938 | 1.00 22.03 | С |
|--------------|--------------|----------|-----|----------------|------------------|------------------|------------------|--------------------------|-----|
| MOTA | 1389 | 0 | PHE | B2062 | -2.303 | 21.655 | 25.022 | 1.00 22.28 | 0 |
| MOTA | 1390 | N | SER | B2063 | -3.183 | 21.406 | 22.970 | 1.00 22.94 | N |
| ATOM | 1391 | CA | | B2063 | -3.403 | 19.972 | 23.135 | 1.00 24.34 | С |
| ATOM | 1392 | CB | | B2063 | -4.120 | 19.379 | 21.921 | 1.00 24.96 | С |
| ATOM | 1393 | OG | | B2063 | -5.510 | 19.618 | 21.995 | 1.00 26.96 | 0 |
| ATOM | 1394 | C | | B2063 | -2.089 | 19.231 | 23.338 | 1.00 24.82 | С |
| ATOM | 1395 | 0 | | B2063 | -2.053 | 18.192 | 23.989 | 1.00 24.78 | 0 |
| ATOM | 1396 | N | | B2064 | -1.010 | 19.754 | 22.778 | 1.00 24.97 | N |
| ATOM | 1397 | CA | | B2064 | 0.266 | 19.091 | 22.952 | 1.00 26.19 | C |
| ATOM | 1398 | CB- | | B2064 | 1.201 | 19.454 | 21.802 | 1.00 25.92 | C |
| ATOM ATOM | 1399 1400 | CG CD | | B2064 B2064 | 0.723 1.437 | 18.846 19.406 | 20.496 19.293 | 1.00 26.10 1.00 26.40 | C |
| ATOM | 1401 | CE | | B2064 B2064 | 2.890 | 19.406 | 19.272 | 1.00 25.79 | C |
| ATOM | 1401 | NZ | | B2064 | 3.444 | 19.339 | 17.935 | 1.00 26.57 | Ŋ |
| ATOM | 1403 | C | | B2064 | 0.860 | 19.447 | 24.312 | 1.00 27.18 | Č |
| ATOM | 1404 | Ö | | B2064 | 1.443 | 18.593 | 24.978 | 1.00 27.11 | Ö |
| ATOM | 1405 | И | | B2065 | 0.680 | 20.696 | 24.734 | 1.00 28.10 | N |
| ATOM | 1406 | CA | | B2065 | 1.175 | 21.142 | 26.030 | 1.00 29.62 | c c |
| ATOM | 1407 | CB | | B2065 | 0.851 | 22.617 | 26.241 | 1.00 29.09 | c |
| ATOM | 1408 | C | | B2065 | 0.520 | 20.309 | 27.128 | 1.00 30.86 | č |
| ATOM | 1409 | 0 | | B2065 | 1.121 | 20.062 | 28.170 | 1.00 30.13 | ō |
| ATOM | 1410 | N | | B2066 | -0.721 | 19.890 | 26.892 | 1.00 32.95 | N |
| ATOM | 1411 | CA | | B2066 | -1.449 | 19.079 | 27.866 | 1.00 35.41 | C |
| ATOM | 1412 | CB | | B2066 | -2.957 | 19.167 | 27.626 | 1.00 35.78 | С |
| ATOM | 1413 | CG | MET | B2066 | -3.588 | 20.479 | 28.047 | 1.00 36.88 | С |
| ATOM | 1414 | SD | MET | B2066 | -3.734 | 20.673 | 29.828 | 1.00 38.18 | S |
| MOTA | 1415 | CE | MET | B2066 | -5.497 | 20.288 | 30.048 | 1.00 38.92 | С |
| ATOM | 1416 | С | MET | B2066 | -1.010 | 17.621 | 27.783 | 1.00 36.81 | С |
| ATOM | 1417 | 0 | MET | B2066 | -1.414 | 16.797 | 28.595 | 1.00 36.82 | 0 |
| ATOM | 1418 | N | GLY | B2067 | -0.178 | 17.311 | 26.798 | 1.00 38.52 | N |
| MOTA | 1419 | CA | GLY | B2067 | 0.292 | 15.950 | 26.644 | 1.00 41.07 | С |
| MOTA | 1420 | C | GLY | B2067 | -0.794 | 14.998 | 26.187 | 1.00 42.84 | С |
| ATOM | 1421 | 0 | | B2067 | -1.321 | 14.214 | 26.979 | 1.00 43.50 | 0 |
| MOTA | 1422 | N | | B2068 | -1.140 | | 24.908 | 1.00 44.30 | N |
| MOTA | 1423 | CA | | B2068 | -2.152 | 14.206 | 24.322 | 1.00 45.93 | C |
| ATOM | 1424 | CB | | B2068 | -3.410 | | 23.903 | 1.00 45.92 | C |
| ATOM | 1425 | OG1 | | B2068 | -3.075 | 15.921 | 22.861 | 1.00 46.12 | 0 |
| ATOM | 1426 | | | B2068 | -3.972 | | 25.093 | 1.00 46.09 | C |
| ATOM ATOM | 1427 1428 | С О | | B2068 B2068 | -1.501 -2.151 | 13.593 12.918 | 23.088 | 1.00 47.07 1.00 47.09 | 0 |
| ATOM | 1429 | N | | B2069 | -0.202 | | 22.257 | 1.00 47.03 | N |
| ATOM | 1430 | CA | | B2069 | 0.599 | | 21.853 | 1.00 40.33 | C |
| ATOM | 1431 | C | | B2069 | -0.085 | | 20.503 | 1.00 50.67 | č |
| ATOM | 1432 | Õ | | B2069 | -0.047 | | 19.741 | 1.00 51.10 | Õ |
| ATOM | 1433 | N | | B2070 | -0.699 | | 20.208 | 1.00 51.17 | N |
| ATOM | 1434 | CA | | B2070 | -1.405 | | 18.952 | 1.00 51.53 | C |
| ATOM | 1435 | CB | | B2070 | -1.574 | | 18.668 | 1.00 51.94 | Ċ |
| ATOM | 1436 | | | B2070 | -0.221 | | 18.341 | 1.00 51.87 | C |
| ATOM | 1437 | | | B2070 | -2.217 | | 19.882 | 1.00 52.15 | C |
| ATOM | 1438 | | | B2070 | -2.470 | | 19.712 | 1.00 52.43 | С |
| ATOM | 1439 | С | | B2070 | -2.792 | | 18.979 | 1.00 51.42 | С |
| MOTA | 1440 | 0 | | B2070 | -3.074 | | 18.232 | 1.00 51.57 | 0 |
| ATOM | 1441 | N | SER | B2071 | -3.653 | | 19.847 | 1.00 51.02 | N |
| ATOM | 1442 | CA | | B2071 | -5.013 | | 19.967 | 1.00 50.61 | C |
| ATOM | 1443 | CB | | B2071 | -5.803 | | 20.938 | 1.00 50.61 | С |
| MOTA | 1444 | OG | SER | B2071 | -5.007 | 11.299 | 22.044 | 1.00 50.73 | 0 |
| | | | | | | | | | |

| ATOM | 1445 | С | SER | B2071 | -5.064 | 14.030 | 20.404 | 1.00 50.07 | С |
|--------------|--------------|---------|-----|----------------|--------------------|------------------|------------------|--------------------------|--------|
| MOTA | 1446 | 0 | SER | B2071 | -4.042 | 14.625 | 20.771 | 1.00 49.91 | 0 |
| MOTA | 1447 | N | LYS | B2072 | -6.258 | 14.612 | 20.340 | 1.00 49.03 | N |
| ATOM | 1448 | CA | | B2072 | -6.440 | 16.004 | 20.728 | 1.00 47.71 | С |
| MOTA | 1449 | CB | LYS | B2072 | -6.637 | 16.898 | 19.495 | 1.00 48.58 | С |
| MOTA | 1450 | CG | | B2072 | -5.733 | 16.597 | 18.312 | 1.00 49.59 | С |
| MOTA | 1451 | CD | LYS | B2072 | -6.215 | 17.358 | 17.087 | 1.00 50.30 | С |
| ATOM | 1452 | CE | | B2072 | -5.500 | 16.909 | 15.820 | 1.00 50.97 | С |
| ATOM | 1453 | NZ | | B2072 | -6.051 | 17.588 | 14.610 | 1.00 51.33 | N |
| MOTA | 1454 | С | | B2072 | -7.670 | 16.146 | 21.610 | 1.00 46.22 | С |
| MOTA | 1455 | 0 | | B2072 | -8.484 | 15.229 | 21.742 | 1.00 46.03 | 0 |
| ATOM | 1456 | N | | B2073 | -7.787 | 17.322 | 22.208 | 1.00 44.70 | N |
| ATOM | 1457 | CA | | B2073 | -8.915 | 17.658 | 23.048 | 1.00 42.68 | C |
| ATOM | 1458 | CB | | B2073 | -8.540 | 18.812 | 23.975 | 1.00 42.47 | C |
| ATOM | 1459 | CG | | B2073 | -7.416 | 18.504 | 24.959 | 1.00 42.08 | C |
| ATOM | 1460 | | | B2073 | -6.916 | 19.781 | 25.594 | 1.00 42.04 | C |
| ATOM | 1461 | | | B2073 | -7.925 | 17.543 | 26.010 | 1.00 42.14 | C |
| MOTA | 1462 | C | | B2073 | -9.999 | 18.116 | 22.083 | 1.00 41.35 | C |
| ATOM | 1463 | 0 | | B2073 | -9.750 | 18.273 | 20.881 | 1.00 41.21 1.00 39.49 | 0 |
| MOTA | 1464 | N | | B2074 | -11.203 | 18.312 | 22.595 | | N C |
| ATOM | 1465 1466 | CA | | B2074 B2074 | -12.252 -11.852 | 18.791 20.211 | 21.727 21.364 | 1.00 37.51 1.00 35.85 | C |
| ATOM ATOM | 1467 | C O | | B2074 B2074 | -11.493 | 20.211 | 22.240 | 1.00 35.43 | 0 |
| ATOM | 1468 | N | | B2074 | -11.878 | 20.548 | 20.082 | 1.00 33.43 | N |
| ATOM | 1469 | CA | | B2075 | -11.524 | 21.900 | 19.704 | 1.00 33.03 | C |
| ATOM | 1470 | CB | | B2075 | -11.287 | 21.990 | 18.194 | 1.00 32.41 | C |
| ATOM | 1471 | CG | | B2075 | -9.846 | 21.778 | 17.802 | 1.00 32.43 | c |
| ATOM | 1472 | | | B2075 | -8.952 | 21.151 | 18.682 | 1.00 32.07 | Č |
| ATOM | 1473 | | | B2075 | -9.379 | 22.191 | 16.557 | 1.00 33.06 | č |
| ATOM | 1474 | | | B2075 | -7.616 | 20.941 | 18.326 | 1.00 33.27 | Č |
| MOTA | 1475 | | | B2075 | -8.047 | 21.987 | 16.187 | 1.00 33.20 | Ċ |
| ATOM | 1476 | CZ | | B2075 | 163. ל- | 21.360 | 17.071 | 1.00 33.45 | С |
| ATOM | 1477 | C | | B2075 | -12.597 | 22.877 | 20.163 | 1.00 31.04 | С |
| ATOM | 1478 | 0 | | B2075 | -12.340 | 24.072 | 20.277 | 1.00 30.78 | 0 |
| ATOM | 1479 | N | GLN | B2076 | -13.787 | 22.357 | 20.462 | 1.00 29.52 | N |
| ATOM | 1480 | CA | GLN | B2076 | -14.897 | 23.185 | 20.929 | 1.00 28.06 | C |
| ATOM | 1481 | CB | GLN | B2076 | -16.226 | 22.493 | 20.630 | 1.00 27.83 | C |
| ATOM | 1482 | CG | GLN | B2076 | -16.489 | 22.365 | 19.144 | 1.00 27.93 | С |
| ATOM | 1483 | CD | GLN | B2076 | -16.666 | 23.716 | 18.479 | 1.00 28.25 | C |
| MOTA | 1484 | | | .B2076 | -16.170 | 23.950 | 17.376 | 1.00 28.52 | 0 |
| MOTA | 1485 | NE2 | GLN | B2076 | | 24.613 | 19.145 | 1.00 27.92 | N |
| MOTA | 1486 | С | GLN | B2076 | -14.765 | 23.476 | 22.423 | 1.00 27.11 | C |
| ATOM | 1487 | 0 | | B2076 | -15.536 | 24.241 | 23.000 | 1.00 26.54 | 0 |
| MOTA | 1488 | N | | B2077 | -13.768 | 22.860 | 23.037 | 1.00 26.23 | N |
| MOTA | 1489 | CA | | B2077 | -13.505 | 23.059 | 24.447 | 1.00 26.09 | C |
| ATOM | 1490 | CB | | B2077 | -13.173 | 21.721 | 25.108 | 1.00 27.19 | C |
| ATOM | 1491 | CG | | B2077 | -14.401 | 20.856 | 25.292 | 1.00 28.36 | C |
| ATOM | 1492 | | | B2077 | -15.304 | 21:276 | 26.043 | 1.00 29.34 | . 0 |
| ATOM | 1493 | | | B2077 | -14.469 | 19.767 | 24.686 | 1.00 29.83 | 0 |
| ATOM | 1494 | C | | B2077 | -12.354 | 24.041 | 24.614 25.730 | 1.00 24.96 1.00 24.58 | C 0 |
| ATOM ATOM | 1495 1496 | 0 | | B2077 | -11.917 -11.870 | 24.328 24.553 | 23.490 | 1.00 24.58 | N |
| ATOM | 1496 | N CA | | B2078 | -10.783 | 25.507 | 23.490 | 1.00 23.44 | C |
| ATOM | 1497 | CB | | B2078 | -9.534 | 24.900 | 22.868 | 1.00 22.63 | c |
| ATOM | 1499 | CG | | B2078 | -8.989 | 23.599 | 23.468 | 1.00 22.02 | C |
| MOTA | 1500 | | | B2078 | -7.933 | 23.010 | 22.543 | 1.00 22.73 | C |
| ATOM | 1501 | | | B2078 | -8.401 | 23.870 | 24.841 | 1.00 22.96 | Č |
| | | | | | 001 | 20.0.0 | | 3.00 20.50 | o o |

| ATOM | 1502 | С | LEU | B2078 | -11.200 | 26.741 | 22.726 | 1.00 22.37 | С |
|------|------|-----------|-----|-------|-------------------|--------|--------|------------|-----|
| MOTA | 1503 | 0 | LEU | B2078 | -11.709 | 26.642 | 21.611 | 1.00 21.73 | 0 |
| MOTA | 1504 | N | GLU | B2079 | -11.001 | 27.908 | 23.324 | 1.00 21.99 | N |
| ATOM | 1505 | CA | GLU | B2079 | -11.342 | 29.145 | 22.648 | 1.00 21.60 | С |
| ATOM | 1506 | CB | GLU | B2079 | -12.624 | 29.740 | 23.214 | 1.00 21.69 | C |
| ATOM | 1507 | CG | | B2079 | -13.132 | 30.922 | 22.421 | 1.00 22.30 | С |
| ATOM | 1508 | CD | | B2079 | -14.459 | 31.412 | 22.937 | 1.00 23.08 | Ċ |
| ATOM | 1509 | | | B2079 | -14.499 | 31.893 | 24.089 | 1.00 24.19 | Ö |
| ATOM | 1510 | | | B2079 | -15.462 | 31.311 | 22.201 | 1.00 22.86 | Ö |
| ATOM | 1511 | C | | B2079 | -10.216 | 30.144 | 22.792 | 1.00 21.14 | č |
| ATOM | 1512 | o | | B2079 | -9.606 | 30.265 | 23.862 | 1.00 21.43 | Ö |
| ATOM | 1513 | N | | B2073 | -9.940 | 30.852 | 21.705 | 1.00 20.42 | N |
| ATOM | 1514 | CA | | B2080 | -8.892 | 31.850 | 21.691 | 1.00 20.15 | C |
| ATOM | 1515 | CB | | B2080 | -7.728 | 31.418 | 20.780 | 1.00 19.96 | c |
| MOTA | 1516 | | | B2080 | -6.662 | 32.517 | 20.735 | 1.00 19.66 | C |
| MOTA | 1517 | | | B2080 | -7.127 | 30.123 | 21.297 | 1.00 19.86 | Ċ |
| MOTA | 1518 | C | | B2080 | -9.436 | 33.187 | 21.211 | 1.00 20.63 | C |
| MOTA | 1519 | 0 | | B2080 | -9.899 | 33.320 | 20.075 | 1.00 20.05 | 0 |
| | 1520 | | | B2081 | -9.379 | 34.178 | 22.089 | 1.00 20.91 | N |
| ATOM | | N | | B2081 | • | | 21.767 | | . C |
| ATOM | 1521 | CA | | | -9.852 -10.913 | 35.515 | | 1.00 21.71 | C |
| ATOM | 1522 | CB | | B2081 | -10.913 | 35.953 | 22.779 | 1.00 21.41 | |
| ATOM | 1523 | CG CD1 | | B2081 | -12.150 | 35.049 | 22.846 | 1.00 21.70 | C |
| ATOM | 1524 | | | B2081 | -13.145 | 35.618 | 23.864 | 1.00 20.86 | C |
| ATOM | 1525 | | | B2081 | -12.788 | 34.947 | 21.451 | 1.00 20.91 | C |
| MOTA | 1526 | С | | B2081 | -8.690 | 36.488 | 21.802 | 1.00 21.95 | C |
| MOTA | 1527 | 0 | | B2081 | -7.592 | 36.135 | 22.255 | 1.00 22.11 | 0 |
| ATOM | 1528 | N | | B2082 | -8.927 | 37.700 | 21.302 | 1.00 22.09 | N |
| ATOM | 1529 | CA | | B2082 | -7.912 | 38.754 | 21.334 | 1.00 22.53 | C |
| MOTA | 1530 | CB | | B2082 | -7.809 | 39.483 | 19.992 | 1.00 23.53 | ·C |
| ATOM | 1531 | CG | | B2082 | -7.347 | 38.588 | 18.882 | 1.00 24.84 | C |
| MOTA | 1532 | | | B2082 | -6.350 | 37.880 | 19.016 | 1.00 25.89 | 0 |
| ATOM | 1533 | | | B2082 | -8.066 | 38.613 | 17.766 | 1.00 26.27 | N |
| MOTA | 1534 | С | | B2082 | -8.345 | 39.754 | 22.402 | 1.00 22.18 | C |
| ATOM | 1535 | 0 | | B2082 | -9.528 | 40.069 | 22.514 | 1.00 21.35 | 0 |
| MOTA | 1536 | N | | B2083 | -7.391 | 40.244 | 23.186 | 1.00 22.35 | N |
| ATOM | 1537 | CA | | B2083 | -7.699 | 41.215 | 24.227 | 1.00 22.53 | C |
| MOTA | 1538 | CB | | B2083 | -6.711 | 41.092 | 25.391 | 1.00 21.65 | C |
| MOTA | 1539 | CG | | B2083 | -5.267 | 41.394 | 24.995 | 1.00 21.91 | C |
| MOTA | 1540 | | | B2083 | -4.338 | 41.115 | 25.762 | 1.00 22.04 | 0 |
| MOTA | 1541 | | | B2083 | -5.068 | 41.963 | 23.808 | 1.00 20.96 | N |
| ATOM | 1542 | С | | B2083 | -7.679 | 42.632 | 23.663 | 1.00 23.31 | C |
| ATOM | 1543 | 0 | | B2083 | -7.344 | 42.834 | 22.493 | 1.00 23.42 | 0 |
| ATOM | 1544 | N | | B2084 | -8.037 | 43.605 | 24.498 | 1.00 23.94 | N |
| ATOM | 1545 | CA | | B2084 | -8.062 | 45.012 | 24.098 | 1.00 24.84 | C |
| ATOM | 1546 | CB | | B2084 | -8.089 | 45.924 | 25.336 | 1.00 26.09 | C |
| ATOM | 1547 | CG | | B2084 | -9.171 | 45.622 | 26.355 | 1.00 28.21 | C |
| ATOM | 1548 | CD | | B2084 | -8.992 | 44.259 | 27.014 | 1.00 30.57 | C |
| ATOM | 1549 | | | B2084 | -7.892 | 44:001 | 27.565 | 1.00 31.38 | 0 |
| ATOM | 1550 | | | B2084 | -9.952 | 43.448 | 26.984 | 1.00 31.36 | 0 |
| ATOM | 1551 | C | | B2084 | -6.871 | 45.421 | 23.223 | 1.00 24.40 | C |
| ATOM | 1552 | 0 | | B2084 | -7.033 | 46.197 | 22.292 | 1.00 24.89 | 0 |
| ATOM | 1553 | N Gr | | B2085 | -5.683 | 44.905 | 23.530 | 1.00 24.24 | N |
| ATOM | 1554 | CA | | B2085 | -4.464 | 45.245 | 22.782 | 1.00 24.07 | C |
| MOTA | 1555 | CB | | B2085 | -3.237 | 45.139 | 23.688 | 1.00 24.81 | C |
| ATOM | 1556 | CG | | B2085 | -3.375 | 45.824 | 25.022 | 1.00 26.63 | C |
| ATOM | 1557 | CD | | B2085 | -2.090 | 45.727 | 25.844 | 1.00 27.63 | C |
| MOTA | 1558 | NE | AKG | B2085 | -2.124 | 46.668 | 26.962 | 1.00 28.81 | N |
| | | | | | | | | | |

| ATOM | 1559 | CZ | | B2085 | -2.915 | 46.532 | 28.016 | 1.00 29.08 | С |
|------|--------------|-----|-----|-------|---------|--------|---------------|------------|-----|
| ATOM | 1560 | | | B2085 | -3.725 | 45.489 | 28.090 | 1.00 30.38 | N |
| MOTA | 1561 | NH2 | ARG | B2085 | -2.915 | 47.441 | 28.984 | 1.00 29.49 | N |
| ATOM | 1562 | С | ARG | B2085 | -4.201 | 44.386 | 21.548 | 1.00 23.45 | С |
| ATOM | 1563 | 0 | ARG | B2085 | -3.231 | 44.616 | 20.839 | 1.00 23.48 | 0 |
| ATOM | 1564 | N | GLY | B2086 | -5.043 | 43.388 | 21.304 | 1.00 22.86 | N |
| ATOM | 1565 | CA | GLY | B2086 | -4.845 | 42.531 | 20.148 | 1.00 22.18 | С |
| ATOM | 1566 | С | | B2086 | -4.106 | 41.231 | 20.442 | 1.00 22.02 | С |
| ATOM | 1567 | 0 | | B2086 | -3.935 | 40.391 | 19.557 | 1.00 22.97 | 0 |
| ATOM | 1568 | N | | B2087 | -3.658 | 41.053 | 21.677 | 1.00 20.91 | N |
| ATOM | 1569 | CA | | B2087 | -2.948 | 39.836 | 22.038 | 1.00 19.91 | С |
| ATOM | 1570 | CB | | B2087 | -2.196 | 40.028 | 23.362 | 1.00 19.31 | · c |
| ATOM | 1571 | C | | B2087 | -3.940 | 38.675 | 22.161 | 1.00 19.35 | Č |
| ATOM | 1572 | 0 | | B2087 | -5.013 | 38.816 | 22.757 | 1.00 18.31 | ō |
| ATOM | 1573 | N | | B2088 | -3.598 | 37.520 | 21.566 | 1.00 19.16 | N |
| ATOM | 1574 | CD | | B2088 | -2.449 | 37.320 | 20.656 | 1.00 19.16 | c |
| ATOM | 1575 | CA | | B2088 | -4.450 | 36.331 | 21.611 | 1.00 18.85 | c |
| | 1576 | | | B2088 | -3.968 | 35.529 | 20.408 | 1.00 19.28 | c |
| ATOM | | CB | | B2088 | -2.478 | 35.817 | 20.403 | 1.00 13.20 | C |
| ATOM | 1577 | CG | | | -4.229 | 35.597 | 22.934 | 1.00 18.72 | C |
| MOTA | 1578 1579 | C . | | B2088 | | 35.484 | | 1.00 18.70 | 0 |
| ATOM | | 0 , | | B2088 | -3.098 | 35.108 | 23.404 23.533 | 1.00 18.33 | N |
| ATOM | 1580 | N | | B2089 | -5.310 | | | | C |
| MOTA | 1581 | CA | | B2089 | -5.230 | | 24.804 | 1.00 17.56 | C |
| ATOM | 1582 | CB | | B2089 | -5.394 | 35.379 | 25.960 | 1.00 15.80 | |
| ATOM | 1583 | CG | | B2089 | -6:792 | 35.933 | 26.103 | 1.00 14.62 | C |
| ATOM | 1584 | | | B2089 | -7.684 | 35.402 | 27.036 | 1.00 14.04 | C |
| ATOM | 1585 | | | B2089 | -8.983 | 35.916 | 27.160 | 1.00 13.45 | C |
| ATOM | 1586 | | | B2089 | -7.231 | 36.991 | 25.294 | 1.00 13.76 | C |
| MOTA | 1587 | | | B2089 | -8.507 | 37.499 | 25.405 | 1.00 12.48 | C |
| ATOM | 1588 | CZ | | B2089 | -9.381 | 36.964 | 26.336 | 1.00 13.07 | C |
| MOTA | 1589 | ОН | | B2089 | -10.649 | 37.475 | 26.433 | 1.00 12.87 | 0 |
| ATOM | 1590 | С | | B2089 | -6.333 | 33.349 | 24.865 | 1.00 18.14 | C |
| MOTA | 1591 | 0 | | B2089 | -7.302 | 33.433 | 24.118 | 1.00 18.32 | 0 |
| MOTA | 1592 | N | | B2090 | -6.196 | 32.360 | 25.741 | 1.00 18.75 | N |
| ATOM | 1593 | CA | | B2090 | -7.242 | 31.350 | 25.853 | 1.00 19.41 | C |
| MOTA | 1594 | CB. | | B2090 | -6.686 | 30.012 | 26.353 | 1.00 18.52 | C |
| ATOM | 1595 | CG | | B2090 | -6.044 | 29.187 | 25.282 | 1.00 18.19 | C |
| MOTA | 1596 | | | B2090 | -4.716 | 29.402 | 24.912 | 1.00 17.08 | С |
| ATOM | 1597 | | | B2090 | -6.769 | 28.182 | 24.638 | 1.00 17.63 | C |
| ATOM | 1598 | | | B2090 | -4.119 | 28.626 | 23.920 | 1.00 16.47 | C |
| MOTA | 1599 | | | B2090 | -6.177 | 27.400 | 23.640 | 1.00 16.79 | C |
| MOTA | 1600 | CZ | | B2090 | -4.847 | 27.625 | 23.284 | 1.00 16.73 | C |
| ATOM | 1601 | С | | B2090 | -8.334 | 31.806 | 26.802 | 1.00 20.35 | C |
| ATOM | 1602 | 0 | | B2090 | -8.092 | 31.963 | 27.997 | 1.00 20.62 | 0 |
| ATOM | 1603 | N | | B2091 | -9.535 | 32.010 | 26.271 | 1.00 21.43 | N |
| MOTA | 1604 | CA | | B2091 | -10.664 | 32.430 | 27.096 | 1.00 22.72 | C |
| ATOM | 1605 | CB | | B2091 | -11.635 | 33.293 | 26.278 | 1.00 22.59 | C |
| ATOM | 1606 | OG | | B2091 | -12.173 | 32:566 | 25.187 | 1.00 24.06 | 0 |
| MOTA | 1607 | С | | B2091 | -11.385 | 31.194 | 27.651 | 1.00 23.50 | С |
| MOTA | 1608 | 0 | | B2091 | -12.133 | 31.289 | 28.623 | 1.00 23.39 | 0 |
| ATOM | 1609 | N | | B2092 | -11.154 | 30.041 | 27.024 | 1.00 24.05 | N |
| MOTA | 1610 | CA | | B2092 | -11.757 | 28.784 | 27.458 | 1.00 25.18 | C |
| ATOM | 1611 | CB | | B2092 | -12.970 | 28.420 | 26.591 | 1.00 26.15 | . C |
| MOTA | 1612 | CG | | B2092 | -14.194 | 29.321 | 26.733 | 1.00 28.02 | C |
| MOTA | 1613 | CD | | B2092 | -14.848 | 29.241 | 28.105 | 1.00 29.69 | C |
| MOTA | 1614 | | | B2092 | -14.974 | 28.159 | 28.687 | 1.00 30.83 | 0 |
| MOTA | 1615 | NE2 | GLN | B2092 | -15.283 | 30.389 | 28.622 | 1.00 30.35 | N |
| | | | | | | | | | |

| ATOM | 1616 | С | GLN | B2092 | • | -10.725 | 27.661 | 27.354 | 1.00 2 | 25.31 | С |
|------|------|-----|-----|-------|---|---------|--------|--------|--------|-------|---|
| MOTA | 1617 | 0 | | B2092 | | -10.029 | 27.541 | 26.343 | 1.00 2 | | 0 |
| ATOM | 1618 | N | | B2093 | • | -10.631 | 26.838 | 28.395 | 1.00 2 | | N |
| ATOM | 1619 | CA | | B2093 | | -9.680 | 25.733 | 28.394 | 1.00 2 | | C |
| ATOM | 1620 | CB | | | | -8.243 | 26.278 | 28.384 | 1.00 2 | | C |
| | | | | B2093 | | | | | | | |
| ATOM | 1621 | C | | B2093 | | -9.876 | 24.805 | 29.587 | 1.00 2 | | С |
| MOTA | 1622 | 0 | | B2093 | | -10.200 | 25.252 | 30.687 | 1.00 2 | | 0 |
| ATOM | 1623 | N | | B2094 | | -9.671 | 23.492 | 29.382 | 1.00 | | N |
| ATOM | 1624 | CD | | B2094 | | -9.377 | 22.840 | 28.090 | 1.00 2 | | С |
| MOTA | 1625 | CA | PRO | B2094 | | -9.824 | 22.497 | 30.452 | 1.00 2 | 28.17 | С |
| MOTA | 1626 | CB | PRO | B2094 | | -9.970 | 21.191 | 29.681 | 1.00 2 | 27.97 | С |
| MOTA | 1627 | CG | PRO | B2094 | | -9.068 | 21.408 | 28.501 | 1.00 2 | 27.75 | С |
| MOTA | 1628 | С | PRO | B2094 | | -8.611 | 22.489 | 31.384 | 1.00 2 | 28.93 | С |
| MOTA | 1629 | 0 | PRO | B2094 | | -8.149 | 21.429 | 31.819 | 1.00 | 29.42 | 0 |
| ATOM | 1630 | N | PHE | B2095 | | -8.099 | 23.676 | 31.690 | 1.00 | 29.04 | N |
| ATOM | 1631 | CA | PHE | B2095 | | -6.929 | 23.812 | 32.551 | 1.00 | 28.93 | С |
| ATOM | 1632 | CB | | B2095 | | -5.704 | 24.150 | 31.689 | 1.00 | | С |
| ATOM | 1633 | CG | | B2095 | | -4.416 | 24.266 | 32.460 | 1.00 | | C |
| ATOM | 1634 | | | B2095 | | -3.697 | 25.457 | 32.454 | 1.00 | | C |
| MOTA | 1635 | | | B2095 | | -3.918 | 23.185 | 33.187 | 1.00 | | C |
| ATOM | 1636 | | | B2095 | | -2.503 | 25.574 | 33.158 | 1.00 | | C |
| ATOM | 1637 | | | B2095 | | -2.730 | 23.292 | 33.893 | 1.00 | | C |
| | | | | | | -2.018 | 24.492 | 33.880 | 1.00 | | c |
| ATOM | 1638 | CZ | | B2095 | | | | | 1.00 | | C |
| ATOM | 1639 | .C | | B2095 | | -7.220 | 24.934 | 33.544 | | | |
| ATOM | 1640 | 0 | | B2095 | | -7.922 | 25.893 | 33.211 | 1.00 | | 0 |
| ATOM | 1641 | N | | B2096 | | -6.690 | 24.821 | 34.758 | 1.00 | | N |
| ATOM | 1642 | CA. | | B2096 | | -6.931 | 25.837 | 35.771 | 1.00 | | C |
| ATOM | 1643 | CB | | B2096 | | -7.374 | 25.177 | 37.078 | 1.00 | | C |
| ATOM | 1644 | OG | | B2096 | | -8.489 | 24.328 | 36.859 | 1.00 | | 0 |
| ATOM | 1645 | С | | B2096 | | -5.719 | 26.716 | 36.038 | 1.00 | | C |
| ATOM | 1646 | 0 | | B2096 | | -5.828 | 27.746 | 36.700 | 1.00 | | 0 |
| MOTA | 1647 | N | | B2097 | | -4.563 | 26.318 | 35.526 | 1.00 | | N |
| MOTA | 1648 | CA | | B2097 | | -3.370 | 27.115 | 35.752 | 1.00 | | С |
| ATOM | 1649 | С | | B2097 | | -3.246 | 28.268 | 34.771 | 1.00 | | С |
| ATOM | 1650 | 0 | | B2097 | | -4.224 | 28.686 | 34.155 | 1.00 | | 0 |
| MOTA | 1651 | N | LYS | B2098 | | -2.032 | 28.786 | 34.629 | 1.00 | | N |
| MOTA | 1652 | CA | LYS | B2098 | | -1.786 | 29.886 | 33.707 | 1.00 | 23.16 | С |
| MOTA | 1653 | CB | LYS | B2098 | | -0.656 | 30.789 | 34.212 | 1.00 | 24.15 | С |
| MOTA | 1654 | CG | LYS | B2098 | | -1.025 | 31.639 | 35.408 | 1.00 | 25.14 | С |
| ATOM | 1655 | CD | LYS | B2098 | | 0.036 | 32.693 | 35.659 | 1.00 | 26.88 | С |
| ATOM | 1656 | CE | | B2098 | | -0.288 | 33.524 | 36.895 | 1.00 | 27.83 | C |
| ATOM | 1657 | NZ | LYS | B2098 | | -0.224 | 32.680 | 38.126 | 1.00 | 28.96 | N |
| ATOM | 1658 | С | LYS | B2098 | | -1.406 | 29.332 | 32.353 | 1.00 | 21.88 | С |
| ATOM | 1659 | 0 | LYS | B2098 | | -0.604 | 28.402 | 32.261 | 1.00 | 21.71 | 0 |
| ATOM | 1660 | N | ILE | B2099 | | -1.997 | 29.905 | 31.310 | 1.00 | 20.39 | N |
| ATOM | 1661 | CA | ILE | B2099 | | -1.723 | 29.494 | 29.941 | 1.00 | 19.37 | С |
| ATOM | 1662 | CB | ILE | B2099 | | -3.027 | 29.186 | 29.165 | 1.00 | 19.23 | С |
| ATOM | 1663 | | | B2099 | | -2.695 | 28:629 | 27.779 | | 18.49 | С |
| ATOM | 1664 | CG1 | ILE | B2099 | | -3.878 | 28.182 | 29.950 | 1.00 | 18.74 | С |
| ATOM | 1665 | CD1 | ILE | B2099 | | -5.199 | 27.892 | 29.299 | 1.00 | 18.23 | С |
| ATOM | 1666 | С | | B2099 | | -0.997 | 30.621 | 29.221 | | 18.65 | С |
| ATOM | 1667 | 0 | | B2099 | | -1.570 | 31.683 | 28.973 | | 18.86 | 0 |
| ATOM | 1668 | N | | B2100 | | 0.273 | 30.401 | 28.907 | | 17.78 | N |
| MOTA | 1669 | CA | | B2100 | | 1.043 | 31.407 | 28.195 | | 17.08 | С |
| ATOM | 1670 | CB | | B2100 | | 2.477 | 31.487 | 28.735 | | 15.80 | С |
| ATOM | 1671 | CG | | B2100 | | 2.533 | 31.922 | 30.180 | | 15.68 | С |
| ATOM | 1672 | | | B2100 | | 2.423 | 33.264 | 30.679 | | 15.05 | C |
| | | | | | | | | ,_, | | | |

| ATOM | 1673 | CE2 | TRP | B2100 | 2.466 | 33.189 | 32.093 | 1.00 15.31 | С |
|--------------|------|-----|-----|----------------|--------|--------|------------------|------------|---|
| ATOM | 1674 | | | B2100 | 2.289 | 34.522 | 30.070 | 1.00 15.15 | C |
| ATOM | 1675 | | | B2100 | 2.636 | 31.111 | 31.284 | 1.00 15.45 | c |
| ATOM | 1676 | | | B2100 | 2.595 | 31.868 | 32.432 | 1.00 15.26 | Ŋ |
| ATOM | 1677 | | | B2100 | 2.384 | 34.328 | 32.912 | 1.00 15.02 | Ċ |
| ATOM | 1678 | | | B2100 | 2.204 | 35.658 | 30.883 | 1.00 15.47 | Č |
| ATOM | 1679 | | | B2100 | 2.253 | 35.548 | 32.291 | 1.00 15.54 | C |
| ATOM | 1680 | C | | B2100 | 1.027 | 31.028 | 26.723 | 1.00 13.34 | C |
| ATOM | 1681 | | | B2100 | 1.627 | 30.041 | 26.311 | 1.00 17.10 | Ö |
| | | 0 | | | | 31.821 | 25.937 | 1.00 17.52 | И |
| ATOM ATOM | 1682 | N | | B2101 | 0.314 | | 24.508 | 1.00 17.56 | C |
| | 1683 | CA | | B2101 B2101 | 0.180 | 31.575 | | 1.00 17.38 | C |
| ATOM ATOM | 1684 | CB | | | -1.304 | 31.454 | 24.137 22.635 | 1.00 17.83 | C |
| | 1685 | CG | | B2101 | -1.641 | 31.497 | | | C |
| ATOM | 1686 | | | B2101 | -1.241 | 30.157 | 21.964 | 1.00 17.98 | |
| ATOM | 1687 | | | B2101 | -3.132 | 31.768 | 22.444 | 1.00 17.63 | C |
| ATOM | 1688 | C | | B2101 | 0.789 | 32.685 | 23.681 | 1.00 17.40 | С |
| ATOM | 1689 | 0 | | B2101 | 0.770 | 33.849 | 24.075 | 1.00 17.23 | 0 |
| MOTA | 1690 | N | | B2102 | 1.332 | 32.312 | 22.529 | 1.00 17.67 | N |
| MOTA | 1691 | CA | | B2102 | 1.892 | 33.274 | 21.602 | 1.00 17.46 | C |
| ATOM | 1692 | CB | | B2102 | 3.366 | 33.551 | 21.892 | 1.00 17.36 | С |
| MOTA | 1693 | OG | | B2102 | 3.797 | 34.687 | 21.150 | 1.00 17.27 | 0 |
| MOTA | 1694 | С | | B2102 | 1.731 | 32.739 | 20.185 | 1.00 17.83 | С |
| ATOM | 1695 | 0 | | B2102 | 1.984 | 31.563 | 19.919 | 1.00 17.13 | 0 |
| MOTA | 1696 | N | | B2103 | 1.286 | 33.616 | 19.288 | 1.00 18.64 | N |
| MOTA | 1697 | CA | ILE | B2103 | 1.084 | 33.270 | 17.888 | 1.00 19.37 | С |
| MOTA | 1698 | CB | ILE | B2103 | -0.429 | 33.275 | 17.515 | 1.00 19.72 | С |
| ATOM | 1699 | | | B2103 | -0.625 | 32.778 | 16.079 | 1.00 19.83 | С |
| MOTA | 1700 | CG1 | ILE | B2103 · | -1.213 | 32.382 | 18.480 | 1.00 20.18 | С |
| ATOM | 1701 | | | B2103 | -2.722 | 32.470 | 18.314 | 1.00 20.28 | С |
| ATOM | 1702 | С | ILE | B2103 | 1.813 | 34.299 | 17.014 | 1.00 19.77 | С |
| MOTA | 1703 | 0 | ILE | B2103 | 1.857 | 35.489 | 17.330 | 1.00 18.81 | 0 |
| ATOM | 1704 | N | SER | B2104 | 2.396 | 33.818 | 15.925 | 1.00 20.35 | N |
| MOTA | 1705 | CA | SER | B2104 | 3.096 | 34.673 | 14.974 | 1.00 21.48 | С |
| ATOM | 1706 | CB | SER | B2104 | 4.603 | 34.675 | 15.268 | 1.00 21.45 | С |
| ATOM | 1707 | OG | SER | B2104 | 5.328 | 35.484 | 14.351 | 1.00 21.11 | 0 |
| ATOM | 1708 | С | SER | B2104 | 2.826 | 34.069 | 13.598 | 1.00 22.45 | С |
| ATOM | 1709 | 0 | SER | B2104 | 2.492 | 32.884 | 13.488 | 1.00 22.26 | 0 |
| MOTA | 1710 | N | HIS | B2105 | 2.949 | 34.872 | 12.549 | 1.00 23.91 | N |
| ATOM | 1711 | CA | | B2105 | 2.725 | 34.348 | 11.207 | 1.00 25.44 | С |
| ATOM | 1712 | CB | | B2105 | 1.235 | 34.372 | 10.867 | 1.00 26.52 | С |
| ATOM | 1713 | CG | | B2105 | 0.682 | 35.754 | 10.693 | 1.00 27.10 | С |
| ATOM | 1714 | | HIS | B2105 | 0.353 | 36.451 | 9.577 | 1.00 27.93 | С |
| MOTA | 1715 | | | B2105 | 0.427 | 36.594 | 11.755 | 1.00 27.73 | N |
| ATOM | 1716 | | | B2105 | -0.036 | 37.747 | 11.302 | 1.00 27.61 | С |
| ATOM | 1717 | | | B2105 | -0.091 | 37.686 | 9.984 | 1.00 27.60 | N |
| ATOM | 1718 | C | | B2105 | | | | 1.00 25.84 | С |
| ATOM | 1719 | 0 | | B2105 | 3.836 | 36.274 | 10.303 | 1.00 25.76 | 0 |
| ATOM | 1720 | N | | B2106 | 3.688 | 34:444 | 9.001 | 1.00 26.43 | N |
| ATOM | 1721 | CA | | B2106 | 4.314 | 35.051 | 7.834 | 1.00 27.12 | С |
| ATOM | 1722 | CB | | B2106 | 5.546 | 34.261 | 7.341 | 1.00 27.09 | Ċ |
| ATOM | 1723 | | | B2106 | 5.137 | 32.968 | 6.888 | 1.00 26.88 | ō |
| ATOM | 1724 | | | B2106 | 6.576 | 34.120 | 8.452 | 1.00 27.18 | c |
| ATOM | 1725 | C | | B2106 | 3.213 | 34.953 | 6.777 | 1.00 27.18 | č |
| ATOM | 1726 | 0 | | B2106 | 2.059 | 34.688 | 7.116 | 1.00 27.39 | 0 |
| ATOM | 1727 | N | | B2103 | 3.553 | 35.148 | 5.508 | 1.00 27.85 | n |
| ATOM | 1728 | CA | | B2107 | 2.554 | 35.068 | 4.449 | 1.00 27.83 | C |
| | 1729 | CB | | B2107 B2107 | 3.085 | 35.722 | 3.170 | 0.05 28.14 | C |
| MOTA | 1129 | CB | MOP | D2 T0 1 | 3.003 | 33.122 | ١١ ٢٠٠ | 0.00 20.14 | C |

| ATOM 1730 CG ASP B2107 3.275 37.220 3.316 0.05 28.09 ATOM 1731 ODI ASP B2107 4.422 37.693 3.1177 0.05 28.08 ATOM 1733 C ASP B2107 4.422 37.693 3.177 0.05 28.08 ATOM 1733 C ASP B2107 0.995 33.408 3.664 1.00 28.673 ATOM 1735 N GLN B2108 2.988 32.662 4.392 1.00 28.673 ATOM 1735 CA GLN B2108 2.663 31.272 4.093 1.00 29.21 ATOM 1735 CA GLN B2108 3.753 30.666 3.201 1.00 30.96 ATOM 1737 CB GLN B2108 3.753 30.666 3.201 1.00 32.72 ATOM 1738 CG GLN B2108 5.386 30.967 1.282 1.00 34.84 ATOM 1737 CD GLN B2108 5.386 30.967 1.282 1.00 34.84 ATOM 1740 CDI GLN B2108 5.395 30.201 0.328 1.00 34.84 ATOM 1741 NEZ GLN B2108 5.395 30.201 0.328 1.00 34.84 ATOM 1742 C GLN B2108 1.899 29.337 5.215 1.00 28.68 ATOM 1744 N PHE B2109 3.066 30.741 6.441 1.00 27.66 ATOM 1745 CA PHE B2109 4.860 30.746 6.441 1.00 27.66 ATOM 1746 CB PHE B2109 4.860 30.741 6.441 1.00 27.66 ATOM 1747 CG PHE B2109 4.860 38.387 5.799 1.00 27.11 ATOM 1740 CDI PHE B2109 4.860 38.387 6.875 1.00 27.11 ATOM 1740 CDI PHE B2109 5.577 28.907 5.799 1.00 27.50 ATOM 1750 CDI PHE B2109 5.577 28.907 5.799 1.00 27.50 ATOM 1751 CDI PHE B2109 5.577 28.907 5.799 1.00 27.50 ATOM 1752 CDI PHE B2109 5.575 26.706 4.823 1.275 1.00 28.68 ATOM 1755 CDI PHE B2109 5.575 26.706 4.823 1.275 1.00 28.67 ATOM 1755 CDI PHE B2109 5.575 26.706 4.823 1.00 27.50 ATOM 1755 CDI PHE B2109 5.575 26.706 4.823 1.00 27.50 ATOM 1755 CDI PHE B2109 5.575 26.706 4.823 1.00 27.50 ATOM 1755 CDI PHE B2109 5.045 26.838 7.683 1.00 27.50 ATOM 1755 CDI PHE B2109 2.524 30.648 8.883 1.00 27.50 ATOM 1755 CDI PHE B2109 2.524 30.648 8.883 1.00 27.50 ATOM 1756 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 1.00 27.50 ATOM 1757 CDI PHE B2109 2.5254 30.648 8.883 | | | | | | | | | | |
|--|------|------|-----|-----|-------|--------|--------|--------|------------|---------------|
| ATOM 1732 OD 2 ASP B2107 | MOTA | 1730 | CG | ASP | B2107 | 3.275 | 37.220 | 3.316 | 0.05 28.09 | С |
| ATOM 1733 C ASP B2107 | ATOM | 1731 | ODl | ASP | B2107 | 2.276 | 37.926 | 3.569 | 0.05 28.04 | 0 |
| ATOM 1735 N GLN B2108 | MOTA | 1732 | OD2 | ASP | B2107 | 4.422 | 37.693 | 3.177 | 0.05 28.08 | 0 |
| ATOM 1735 N GLN B2108 2.988 32.662 4.392 1.00 28.69 ATOM 1736 CA GLN B2108 2.663 31.272 4.093 1.00 29.21 ATOM 1737 CB GLN B2108 3.753 30.666 3.201 1.00 30.96 ATOM 1738 CG GLN B2108 3.753 30.666 3.201 1.00 30.96 ATOM 1739 CD GLN B2108 5.386 30.967 1.292 1.00 34.84 ATOM 1740 OEI GLN B2108 6.605 31.306 1.699 1.00 34.84 ATOM 1741 NEZ GLN B2108 6.605 31.306 1.699 1.00 34.84 ATOM 1742 CC GLN B2108 1.819 29.337 5.215 1.00 28.68 ATOM 1743 O GLN B2108 1.819 29.337 5.215 1.00 28.68 ATOM 1744 N PHE B2109 3.068 30.741 6.441 1.00 27.66 ATOM 1745 CA PHE B2109 4.367 29.287 7.953 1.00 26.50 ATOM 1746 CB PHE B2109 4.360 28.387 6.875 1.00 27.11 ATOM 1747 CG PHE B2109 4.860 28.387 6.875 1.00 27.11 ATOM 1748 CD PHE B2109 4.599 27.020 6.913 1.00 26.71 ATOM 1750 CEI PHE B2109 5.575 26.706 4.823 1.00 27.16 ATOM 1751 CEZ PHE B2109 5.045 26.180 5.893 1.00 27.16 ATOM 1753 C PHE B2109 2.524 30.648 8.883 1.00 27.55 ATOM 1754 O PHE B2109 2.524 30.648 8.883 1.00 27.55 ATOM 1755 C PHE B2109 2.524 30.648 8.883 1.00 27.55 ATOM 1756 CA VAL B2110 2.016 29.881 11.00 27.56 ATOM 1757 CB VAL B2110 2.016 29.881 11.267 1.00 23.42 ATOM 1756 CA VAL B2110 2.016 29.881 11.267 1.00 23.42 ATOM 1756 CA VAL B2110 2.021 29.555 30.161 11.276 1.00 23.49 ATOM 1760 C VAL B2110 2.021 29.562 31.872 8.967 1.00 23.49 ATOM 1761 O VAL B2110 2.016 29.881 11.267 1.00 23.49 ATOM 1763 CA THR B2111 2.555 30.161 13.314 1.00 22.56 ATOM 1763 CA THR B2111 2.555 30.161 13.314 1.00 22.56 ATOM 1767 CB VAL B2110 2.021 29.562 12.188 1.00 22.51 ATOM 1767 CB VAL B2110 2.021 29.562 12.188 1.00 23.40 ATOM 1767 CB THR B2111 2.555 30.161 13.314 1.00 23.42 ATOM 1767 CB THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1767 CB THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1767 CB THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1768 CB THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1768 CB THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1768 CB THR B2111 2.555 30.161 13.314 1.00 22.55 ATOM 1768 CB THR B2111 2.555 20.161 10.00 17.74 ATOM 1768 CB THR B2111 2.555 20.161 10.00 17.74 ATOM 1776 CB SER B2113 | ATOM | 1733 | С | ASP | B2107 | 2.116 | 33.632 | 4.138 | 1.00 28.63 | C |
| ATOM 1736 CA GLN B2108 | ATOM | 1734 | 0 | ASP | B2107 | 0.995 | 33.408 | 3.684 | | 0 |
| ATOM 1737 CB GLN B2108 | MOTA | 1735 | N | GLN | B2108 | 2.988 | 32.662 | 4.392 | 1.00 28.69 | N |
| ATOM 1738 CG GLN B2108 | MOTA | | CA | GLN | B2108 | 2.663 | | | 1.00 29.21 | С |
| ATOM 1739 CD GLN B2108 5.386 30.967 1.282 1.00 34.31 ATOM 1740 OEI GLN B2108 5.195 30.201 0.328 1.00 34.84 ATOM 1741 NEZ GLN B2108 6.605 31.306 1.699 1.00 34.84 ATOM 1742 C GLN B2108 2.482 30.366 5.308 1.00 28.68 ATOM 1743 O GLN B2108 1.819 29.337 5.215 1.00 28.89 ATOM 1744 N PHE B2109 2.985 29.916 7.641 1.00 27.66 ATOM 1745 CA PHE B2109 2.985 29.916 7.641 1.00 26.61 ATOM 1746 CB PHE B2109 4.347 29.287 7.953 1.00 26.61 ATOM 1747 CG PHE B2109 4.860 28.387 6.875 1.00 27.11 ATOM 1748 CDI PHE B2109 5.577 28.997 5.799 1.00 27.30 ATOM 1749 CDI PHE B2109 6.026 28.073 4.773 1.00 27.16 ATOM 1749 CDI PHE B2109 6.026 28.073 4.773 1.00 27.16 ATOM 1750 CEI PHE B2109 5.045 26.180 5.893 1.00 26.71 ATOM 1751 CE2 PHE B2109 5.757 26.706 4.823 1.00 27.16 ATOM 1753 C PHE B2109 5.045 26.180 5.893 1.00 27.16 ATOM 1753 C PHE B2109 2.625 31.872 8.967 1.00 27.50 ATOM 1755 C PHE B2109 2.625 31.872 8.967 1.00 27.50 ATOM 1755 C PHE B2109 2.625 31.872 8.967 1.00 27.50 ATOM 1756 CA VAL B2110 2.016 29.881 9.843 1.00 24.04 ATOM 1757 CB VAL B2110 1.580 30.435 11.114 1.00 23.42 ATOM 1758 CGI VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1759 CGZ VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1760 C VAL B2110 2.371 28.364 11.996 1.00 23.349 ATOM 1761 C VAL B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 1.00 25.57 ATOM 1766 C C THR B2111 3.175 29.402 14.390 1.00 22.51 ATOM 1767 C THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1768 O THR B2111 5.315 28.803 15.33 1.00 25.57 ATOM 1767 C C BALB B2110 4.674 29.721 14.459 1.00 23.02 ATOM 1768 CG C RH B2111 4.694 29.721 14.459 1.00 23.02 ATOM 1767 C C BALB B2111 3.175 29.402 14.390 1.00 25.55 ATOM 1767 C C BALB B2111 4.694 29.721 14.459 1.00 23.02 ATOM 1767 C C BALB B2111 3.175 29.402 14.390 1.00 25.55 ATOM 1768 CG C BR B2111 3.654 29.828 17.985 1.00 17.74 ATOM 1769 C SER B2113 3.95 29.402 14.390 1.00 25.55 ATOM 1767 C C BALB B2111 2.535 29.402 14.390 1.00 25.55 ATOM 1768 CG C BALB B2111 2.636 28.349 1.00 16.75 ATOM 1779 C ALA B2112 2.865 28.748 16.649 1.00 17.75 ATOM 17 | MOTA | 1737 | CB | | | 3.753 | 30.666 | | | С |
| ATOM 1740 OE1 CLN B2108 | | 1738 | CG | GLN | B2108 | 4.217 | 31.565 | 2,059 | 1.00 32.72 | , C |
| ATOM 1741 NEZ CLN B2108 | | 1739 | CD | GLN | B2108 | 5.386 | | 1.282 | | С |
| ATOM 1742 C GLN B2108 | | | | | | | 30.201 | | | 0 |
| ATOM 1744 N PHE B2109 3.068 30.741 6.441 1.00 27.66 ATOM 1745 CA PHE B2109 2.985 29.916 7.641 1.00 26.50 ATOM 1746 CB PHE B2109 4.347 29.287 7.953 1.00 26.61 ATOM 1747 CG PHE B2109 4.860 28.387 6.875 1.00 27.11 ATOM 1748 CD1 PHE B2109 4.860 28.387 6.875 1.00 27.11 ATOM 1749 CD2 PHE B2109 4.860 28.387 6.875 1.00 27.11 ATOM 1749 CD2 PHE B2109 4.599 27.020 6.913 1.00 26.71 ATOM 1750 CEI PHE B2109 6.026 28.073 4.773 1.00 27.50 ATOM 1751 CE2 PHE B2109 5.757 28.907 3.799 1.00 27.50 ATOM 1753 C PHE B2109 5.757 26.706 4.823 1.00 27.50 ATOM 1753 C PHE B2109 5.757 26.706 4.823 1.00 27.50 ATOM 1753 C PHE B2109 2.625 31.872 8.967 1.00 25.59 ATOM 1755 N VAL B2110 2.016 29.881 9.843 1.00 25.59 ATOM 1755 N VAL B2110 1.580 30.435 11.267 1.00 23.42 ATOM 1757 CB VAL B2110 0.045 30.435 11.267 1.00 23.42 ATOM 1758 CG1 VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1760 C VAL B2110 2.201 29.562 12.188 1.00 23.49 ATOM 1761 O VAL B2110 2.201 29.562 12.188 1.00 23.38 ATOM 1762 N THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 10.02 2.51 ATOM 1766 CG2 THR B2111 4.674 29.721 14.459 1.00 23.38 ATOM 1766 CG2 THR B2111 4.674 29.721 14.459 1.00 23.10 ATOM 1767 C THR B2111 2.555 30.161 13.314 1.00 23.255 ATOM 1768 CG1 THR B2111 5.310 28.830 15.373 1.00 23.02 ATOM 1769 N ALA B2110 2.956 28.748 16.649 1.00 19.97 ATOM 1760 C THR B2111 4.674 29.721 14.459 1.00 23.10 ATOM 1760 C THR B2111 5.310 28.830 15.373 1.00 25.57 ATOM 1760 CG THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1760 CG THR B2111 3.375 29.402 14.390 1.00 23.02 ATOM 1767 CG BER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1767 CG SER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1770 CG ALA B2112 2.866 28.748 16.649 1.00 19.97 ATOM 1771 CB SER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1776 CB SER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1777 CG SER B2113 2.866 28.749 22.551 1.00 17.74 ATOM 1778 C SER B2113 2.865 28.749 22.551 1.00 17.74 ATOM 1779 C SER B2113 2.865 28.439 22.551 1.00 17.74 ATOM 1779 C SER B2113 2.865 28.439 22.551 1.00 17.60 ATOM 1778 C | | | | | | | | | | N |
| ATOM 1744 N PHE B2109 | | | | | | | | | | С |
| ATOM 1745 CA PHE B2109 | | | | | | | | | | 0 |
| ATOM 1746 CB PHE B2109 | | | | | | | | | | N |
| ATOM 1747 CG PHE B2109 | | | | | | | | | | С |
| ATOM 1748 CD1 PHE B2109 | | | | | | | | | | С |
| ATOM 1749 CD2 PHE B2109 | | | | | | | | | | C |
| ATOM 1750 CE1 PHE B2109 | | | | | | | | | | C |
| ATOM 1751 CE2 PHE B2109 5.045 26.180 5.893 1.00 27.16 ATOM 1752 CZ PHE B2109 5.757 26.706 4.823 1.00 27.50 ATOM 1753 C PHE B2109 2.524 30.648 8.883 1.00 25.59 ATOM 1754 O PHE B2109 2.625 31.872 8.967 1.00 25.67 ATOM 1755 N VAL B2110 2.016 29.881 9.843 1.00 24.04 ATOM 1756 CA VAL B2110 0.045 30.435 11.114 1.00 23.42 ATOM 1757 CB VAL B2110 0.045 30.435 11.1267 1.00 23.14 ATOM 1758 CG1 VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1759 CG2 VAL B2110 -0.327 31.151 12.535 1.00 23.40 ATOM 1760 C VAL B2110 2.201 29.562 12.188 1.00 22.98 ATOM 1761 O VAL B2110 2.371 28.364 11.996 1.00 23.38 ATOM 1762 N THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 1.00 22.51 ATOM 1765 OG1 THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1766 CG2 THR B2111 4.891 31.148 14.928 1.00 23.27 ATOM 1767 C THR B2111 2.531 29.714 15.735 1.00 23.27 ATOM 1768 O THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1771 CB ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1771 CB ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 17.74 ATOM 1774 N SER B2113 2.805 28.227 19.073 1.00 17.74 ATOM 1775 C BER B2113 3.597 28.260 21.365 1.00 17.74 ATOM 1776 C SER B2113 3.597 28.260 21.365 1.00 17.74 ATOM 1777 O SER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1777 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1777 C SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1777 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1778 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1779 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1778 C SER B2113 3.597 28.250 21.365 1.00 17.79 ATOM 1778 C SER B2113 3.597 28.250 21.365 1.00 17.35 ATOM 1780 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1781 CG VAL B2114 0.718 26.533 24.612 1.00 16.65 ATOM 1783 CG VAL B2114 0.718 26.533 24.612 1.00 16.65 | | | | | | | | | | C |
| ATOM 1752 CZ PHE B2109 5.757 26.706 4.823 1.00 27.50 ATOM 1753 C PHE B2109 2.524 30.648 8.883 1.00 25.59 ATOM 1754 O PHE B2109 2.625 31.872 8.967 1.00 25.67 ATOM 1755 N VAL B2110 2.016 29.881 9.843 1.00 24.04 ATOM 1755 CA VAL B2110 1.580 30.435 11.114 1.00 23.42 ATOM 1757 CB VAL B2110 -0.498 29.016 11.276 1.00 23.14 ATOM 1758 CG1 VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1759 CG2 VAL B2110 -0.327 31.151 12.535 1.00 23.49 ATOM 1760 C VAL B2110 2.011 29.562 12.188 1.00 22.98 ATOM 1761 O VAL B2110 2.371 28.364 11.996 1.00 23.38 ATOM 1762 N THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 1.00 22.51 ATOM 1766 CG2 THR B2111 5.310 28.830 15.373 1.00 25.57 ATOM 1766 CG2 THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1766 CG2 THR B2111 2.531 29.714 15.735 1.00 23.27 ATOM 1768 O THR B2111 2.531 29.714 15.735 1.00 23.27 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 23.27 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 17.74 ATOM 1770 CA SALA B2112 2.565 28.748 16.649 1.00 17.74 ATOM 1770 CA SER B2113 3.597 28.250 21.365 1.00 17.74 ATOM 1771 CB SAR B2113 3.597 28.250 21.365 1.00 17.75 ATOM 1773 C SER B2113 3.597 28.250 21.365 1.00 17.75 ATOM 1774 N SER B2113 2.8050 28.839 21.495 1.00 17.75 ATOM 1777 C SER B2113 2.8050 28.839 21.495 1.00 17.75 ATOM 1779 C SER B2113 3.597 28.250 21.365 1.00 17.35 ATOM 1779 C SER B2113 2.8050 28.839 21.495 1.00 17.75 ATOM 1780 C VAL B2114 0.012 26.347 25.999 1.00 16.67 ATOM 1781 CA VAL B2114 0.012 26.347 25.999 1.00 16.16 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 1 | | | | | | | | | | C |
| ATOM 1753 C PHE B2109 2.524 30.648 8.883 1.00 25.59 ATOM 1754 O PHE B2109 2.625 31.872 8.967 1.00 25.67 ATOM 1755 N VAL B2110 2.016 29.881 9.843 1.00 25.67 ATOM 1756 CA VAL B2110 1.580 30.435 11.114 1.00 23.42 ATOM 1757 CB VAL B2110 0.045 30.435 11.114 1.00 23.42 ATOM 1758 CG1 VAL B2110 -0.498 29.016 11.267 1.00 23.49 ATOM 1759 CG2 VAL B2110 -0.327 31.151 12.535 1.00 23.40 ATOM 1760 C VAL B2110 2.201 29.562 12.188 1.00 22.98 ATOM 1761 O VAL B2110 2.371 28.364 11.996 1.00 23.38 ATOM 1761 O VAL B2110 2.371 28.364 11.996 1.00 23.38 ATOM 1762 N THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 1.00 22.51 ATOM 1765 CG1 THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1765 CG1 THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1766 CG2 THR B2111 4.891 31.148 14.928 1.00 23.27 ATOM 1766 CG2 THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.531 29.714 15.735 1.00 21.65 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.357 27.168 18.857 1.00 16.81 ATOM 1775 CA SER B2113 3.597 28.227 19.073 1.00 17.84 ATOM 1777 CB SER B2113 3.597 28.227 19.073 1.00 17.74 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 CB SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 CB SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 CB SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1779 C SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1779 C SER B2113 3.266 29.510 22.905 1.00 17.06 ATOM 1779 C SER B2113 2.860 28.834 20.251 1.00 17.60 ATOM 1779 C SER B2113 2.860 28.834 20.251 1.00 17.60 ATOM 1779 C SER B2113 2.860 28.834 20.251 1.00 17.60 ATOM 1779 C SER B2113 2.262 29.510 22.905 1.00 17.93 ATOM 1779 C SER B2113 2.262 29.510 22.905 1.00 17.93 ATOM 1779 C SER B2113 2.262 29.510 22.905 1.00 17.60 ATOM 1781 CA VAL B2114 2.020 27.383 24.508 1.00 16.65 ATOM 17 | | | | | | | | | | C |
| ATOM 1754 O PHE B2109 | | | | | | | | | | C |
| ATOM 1755 N VAL B2110 2.016 29.881 9.843 1.00 24.04 ATOM 1756 CA VAL B2110 1.580 30.435 11.114 1.00 23.42 ATOM 1757 CB VAL B2110 -0.498 29.016 11.276 1.00 23.49 ATOM 1759 CG2 VAL B2110 -0.327 31.151 12.535 1.00 23.40 ATOM 1759 CG2 VAL B2110 2.201 29.562 12.188 1.00 23.49 ATOM 1760 C VAL B2110 2.201 29.562 12.188 1.00 22.98 ATOM 1761 O VAL B2110 2.371 28.364 11.996 1.00 23.38 ATOM 1762 N THR B2111 2.555 30.161 13.314 1.00 22.66 ATOM 1763 CA THR B2111 3.175 29.402 14.390 1.00 22.51 ATOM 1766 CG2 THR B2111 4.674 29.721 14.459 1.00 23.02 ATOM 1766 CG2 THR B2111 4.891 31.148 14.928 1.00 23.27 ATOM 1766 CG2 THR B2111 2.531 29.714 15.735 1.00 23.27 ATOM 1768 O THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.013 30.807 15.939 1.00 21.65 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1771 CB ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1772 C ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1773 O ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1771 CB ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1772 C ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1773 O ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 CB SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 OG SER B2113 2.860 28.834 20.251 1.00 17.94 ATOM 1777 OG SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1777 OG SER B2113 2.860 28.834 20.251 1.00 17.90 ATOM 1778 C SER B2113 2.860 28.834 20.251 1.00 17.90 ATOM 1779 O SER B2113 2.865 28.439 22.653 1.00 17.35 ATOM 1778 CA VAL B2114 2.749 27.382 23.450 1.00 17.66 ATOM 1781 CA VAL B2114 2.749 27.382 23.450 1.00 16.75 ATOM 1781 CA VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1781 CA VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1785 CC VAL B2114 0.718 26.537 25.999 1.00 16.65 | | | | | | | | | | C |
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| ATOM 1759 CG2 VAL B2110 | | | | | | | | | | C |
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| ATOM 1765 OG1 THR B2111 5.310 28.830 15.373 1.00 25.57 ATOM 1766 CG2 THR B2111 4.891 31.148 14.928 1.00 23.27 ATOM 1767 C THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.013 30.807 15.939 1.00 21.65 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.22 ATOM 1781 CA VAL B2114 2.749 27.382 23.452 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.347 25.999 1.00 16.16 ATOM 1783 CG1 VAL B2114 0.718 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.718 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.718 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 | | | | | | | | | | C |
| ATOM 1766 CG2 THR B2111 4.891 31.148 14.928 1.00 23.27 ATOM 1767 C THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.013 30.807 15.939 1.00 21.65 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 16.72 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1778 C SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.25 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.25 ATOM 1785 C VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | 0 |
| ATOM 1767 C THR B2111 2.531 29.714 15.735 1.00 21.17 ATOM 1768 O THR B2111 2.013 30.807 15.939 1.00 21.65 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 2.805 28.439 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | C |
| ATOM 1768 O THR B2111 2.013 30.807 15.939 1.00 21.65 ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.25 ATOM 1785 C VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | c |
| ATOM 1769 N ALA B2112 2.565 28.748 16.649 1.00 19.97 ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.25 ATOM 1785 C VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | Ö |
| ATOM 1770 CA ALA B2112 1.986 28.928 17.985 1.00 18.49 ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1785 C VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | N |
| ATOM 1771 CB ALA B2112 0.549 28.422 18.009 1.00 16.81 ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1784 CG2 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1785 C VAL B2114 -0.298 27.205 23.675 1.00 17.45 | | | | | | | | | | C |
| ATOM 1772 C ALA B2112 2.805 28.227 19.073 1.00 17.74 ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | | | | | | | | | | C |
| ATOM 1773 O ALA B2112 3.375 27.168 18.857 1.00 16.72 ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | | | | | | | | | | С |
| ATOM 1774 N SER B2113 2.860 28.834 20.251 1.00 17.84 ATOM 1775 CA SER B2113 3.597 28.250 21.365 1.00 17.93 ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | | 1773 | 0 | | | | | | | 0 |
| ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | MOTA | 1774 | N | | | 2.860 | | | | N |
| ATOM 1776 CB SER B2113 4.985 28.893 21.495 1.00 17.90 ATOM 1777 OG SER B2113 5.742 28.263 22.512 1.00 17.60 ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | ATOM | 1775 | CA | SER | B2113 | 3.597 | 28.250 | 21.365 | 1.00 17.93 | С |
| ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | | 1776 | | | | | | | | С |
| ATOM 1778 C SER B2113 2.805 28.439 22.653 1.00 17.35 ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | MOTA | 1777 | OG | SER | B2113 | 5.742 | 28:263 | 22.512 | 1.00 17.60 | 0 |
| ATOM 1779 O SER B2113 2.262 29.510 22.905 1.00 17.22 ATOM 1780 N VAL B2114 2.749 27.382 23.452 1.00 16.89 ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | MOTA | 1778 | С | | | 2.805 | | | | С |
| ATOM 1781 CA VAL B2114 2.020 27.383 24.708 1.00 16.75 ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | MOTA | 1779 | 0 | SER | B2113 | 2.262 | 29.510 | | 1.00 17.22 | 0 |
| ATOM 1782 CB VAL B2114 0.718 26.533 24.612 1.00 16.63 ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | ATOM | 1780 | N | VAL | B2114 | 2.749 | 27.382 | 23.452 | 1.00 16.89 | N |
| ATOM 1783 CG1 VAL B2114 0.112 26.347 25.999 1.00 16.16 ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | MOTA | 1781 | CA | VAL | B2114 | | | | | С |
| ATOM 1784 CG2 VAL B2114 -0.298 27.205 23.675 1.00 16.25 ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | ATOM | 1782 | CB | VAL | B2114 | 0.718 | 26.533 | 24.612 | 1.00 16.63 | С |
| ATOM 1785 C VAL B2114 2.862 26.799 25.835 1.00 17.45 | | | | | | | | | 1.00 16.16 | С |
| | | | CG2 | | | -0.298 | 27.205 | | 1.00 16.25 | С |
| ATOM 1786 O VAL B2114 3.503 25.750 25.680 1.00 16.99 | | | С | | | | | | | С |
| | ATOM | 1786 | 0 | VAL | B2114 | 3.503 | 25.750 | 25.680 | 1.00 16.99 | 0 |

| ATOM | 1787 | N | ILE | B2115 | 2.863 | 27.497 | 26.966 | 1.00 17.80 | N |
|--------------|--------------|-----------|-------|----------------|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 1788 | CA | ILE | B2115 | 3.566 | 27.037 | 28.156 | 1.00 18.72 | С |
| MOTA | 1789 | CB | ILE | B2115 | 4.689 | 28.008 | 28.602 | 1.00 18.37 | С |
| MOTA | 1790 | CG2 | ILE | B2115 | 5.385 | 27.452 | 29.846 | 1.00 18.27 | C |
| MOTA | 1791 | CG1 | ILE | B2115 | 5.708 | 28.205 | 27.480 | 1.00 18.40 | С |
| MOTA | 1792 | CD1 | ILE | B2115 | 6.745 | 29.289 | 27.786 | 1.00 17.55 | С |
| MOTA | 1793 | С | ILE | B2115 | 2.515 | 27.000 | 29.260 | 1.00 19.25 | С |
| ATOM | 1794 | 0 | ILE | B2115 | 1.858 | 28.004 | 29.524 | 1.00 19.38 | 0 |
| MOTA | 1795 | N | LEU | B2116 | 2.336 | 25.846 | 29.884 | 1.00 20.55 | N |
| MOTA | 1796 | CA | | B2116 | 1.374 | 25.735 | 30.968 | 1.00 22.30 | . С |
| MOTA | 1797 | CB | LEU | B2116 | 0.628 | 24.404 | 30.902 | 1.00 21.86 | С |
| MOTA | 1798 | CG | | B2116 | -0.147 | 24.159 | 29.603 | 1.00 22.00 | С |
| MOTA | 1799 | | | B2116 | -0.976 | 22.893 | 29.732 | 1.00 21.49 | С |
| ATOM | 1800 | | | B2116 | -1.050 | 25.359 | 29.303 | 1.00 21.93 | С |
| MOTA | 1801 | С | | B2116 | 2.123 | 25.864 | 32.290 | 1.00 24.11 | C |
| MOTA | 1802 | 0 | | B2116 | 3.209 | 25.299 | 32.472 | 1.00 23.89 | 0 |
| MOTA | 1803 | N | | B2117 | 1.544 | 26.621 | 33.210 | 1.00 26.00 | N |
| MOTA | 1804 | CA | | B2117 | 2.177 | 26.840 | 34.493 | 1.00 28.60 | C |
| ATOM | 1805 | CB | | B2117 | 2.746 | 28,258 | 34.531 | 1.00 28.59 | C |
| ATOM | 1806 | CG | | B2117 | 3.418 | 28.627 | 35.829 | 1.00 30.48 | C |
| MOTA | 1807 | CD | | B2117 | 4.079 | 29.997 | 35.771 | 1.00 31.11 | С |
| ATOM | 1808 | | | B2117 | 3.395 | 30.972 | 35.385 36.115 | 1.00 31.07 1.00 31.14 | 0 |
| ATOM | 1809 | | | B2117 | 5.281 | 30.092 26.601 | | 1.00 31.14 | c |
| ATOM | 1810 | C | | B2117 B2117 | 1.217 0.029 | 26.938 | 35.659 35.595 | 1.00 30.07 | 0 |
| ATOM | 1811 | 0 | | B2117 | 1.742 | 26.006 | 36.726 | 1.00 23.34 | Ŋ |
| ATOM ATOM | 1812 1813 | N | | B2118 | 0.926 | 25.712 | 37.889 | 1.00 34.40 | C |
| ATOM | 1814 | CA CB | | B2118 | 0.997 | 24.223 | 38.212 | 1.00 35.62 | Č |
| ATOM | 1815 | CG | | B2118 | -0.294 | 23.679 | 38.772 | 1.00 37.98 | č |
| ATOM | 1816 | CD | | B2118 | -1.458 | 23.905 | 37.825 | 1.00 37.33 | č |
| ATOM | 1817 | | | B2118 | -1.403 | 23.398 | 36.682 | 1.00 39.94 | Ö |
| ATOM | 1818 | | | B2118 | -2.422 | 24.596 | 38.222 | 1.00 40.32 | Ö |
| ATOM | 1819 | C | | B2118 | 1.387 | 26.515 | 39.090 | 1.00 35.21 | c |
| ATOM | 1820 | ō | | B2118 | 2.611 | 26.552 | 39.343 | 1.00 35.67 | 0 |
| MOTA | 1821 | | | B2118 | 0.507 | 27.088 | 39.767 | 1.00 36.45 | 0 |
| TER | 1822 | | | B2118 | | | | | |
| ATOM | 1823 | CB | | C3003 | 14.254 | 28.191 | 38.580 | 1.00 31.28 | С |
| MOTA | 1824 | CG | MET | C3003 | 15.448 | 27.262 | 38.618 | 1.00 32.93 | С |
| ATOM | 1825 | SD | MET | C3003 | 16.870 | 27.987 | 39.434 | 1.00 35.68 | S |
| ATOM | 1826 | CE | MET | C3003 | 16.438 | 27.672 | 41.140 | 1.00 34.95 | С |
| ATOM | 1827 | С | MET | C3003 | 13.519 | . 27.087 | 36.482 | 1.00 29.25 | С |
| ATOM | 1828 | 0 | MET | C3003 | 13.901 | 25.920 | 36.332 | 1.00 28.76 | 0 |
| ATOM | 1829 | N | | C3003 | 12.435 | 26.519 | 38.666 | 1.00 30.53 | N |
| MOTA | 1830 | CA | | C3003 | 13.052 | 27.596 | 37.845 | 1.00 30.20 | С |
| ATOM | 1831 | N | | C3004 | 13.491 | 27.976 | 35.493 | 1.00 28.16 | N |
| MOTA | 1832 | ĊА | | C3004 | 13.945 | 27.636 | 34.149 | 1.00 27.31 | C |
| MOTA | 1833 | CB | | C3004 | 13.377 | 28.604 | 33.084 | 1.00 27.05 | C |
| MOTA | 1834 | | | C3004 | 14.103 | 28:413 | 31.761 | 1.00 26.26 | C |
| MOTA | 1835 | | | C3004 | 11.876 | 28.372 | 32.919 | 1.00 26.90 | C |
| ATOM | 1836 | | | C3004 | 11.203 | 29.374 | 31.996 | 1.00 27.09 | C |
| ATOM | 1837 | С | | C3004. | | 27.775 | 34.170 | 1.00 26.61 | C |
| ATOM | 1838 | 0 | | C3004 | 15.970 | 28.755 | 34.685 | 1.00 26.80 | 0 |
| MOTA | 1839 | N | | C3005 | 16.153 | 26.794 | 33.617 | 1.00 26.02 | N C |
| ATOM | 1840 | CA | | C3005 C3005 | 17.611 18.221 | 26.822 25.644 | 33.581 34.396 | 1.00 25.10 1.00 25.36 | C |
| ATOM ATOM | 1841 1842 | CB CG1 | | C3005 | 17.820 | 25.766 | 35.869 | 1.00 25.36 | C |
| MOTA | 1843 | | | C3005 | 17.755 | 24.306 | 33.833 | 1.00 23.11 | C |
| VI OU | 1047 | -052 | A 12T | 05003 | 11.133 | 24.500 | JJ. 0JJ | 1.00 23.31 | C |

| MOTA | 1844 | С | VAL | C3005 | 18.124 | 26.747 | 32.152 | 1.00 24.50 | C |
|--------------|--------------|---------|------|---------|------------------|----------|------------------|--------------------------|--------|
| ATOM | 1845 | 0 | VAL | C3005 | 19.327 | 26.640 | 31.928 | 1.00 25.44 | 0 |
| MOTA | 1846 | N | GLY | C3006 | 17.212 | 26.805 | 31.186 | 1.00 23.63 | N |
| MOTA | 1847 | CA | GLY | C3006 | 17.612 | 26.736 | 29.791 | 1.00 22.31 | C |
| ATOM | 1848 | С | GLY | C3006 | 16.446 | 26.762 | 28.820 | 1.00 21.49 | C |
| ATOM | 1849 | 0 | | C3006 | 15.332 | | 29.156 | 1.00 21.47 | 0 |
| ATOM | 1850 | N | HIS | C3007 | 16.700 | 27.254 | 27.609 | 1.00 20.33 | N |
| ATOM | 1851 | CA | HIS | C3007 | 15.664 | 27.336 | 26.582 | 1.00 19.44 | C |
| MOTA | 1852 | CB | HIS | C3007 | 14.806 | | 26.785 | 1.00 18.31 | C |
| MOTA | 1853 | CG | | C3007 | 13.749 | | 25.741 | 1.00 18.22 | C C |
| ATOM | 1854 | | | C3007 | 13.411 | | 24.997 | 1.00 18.17 | Ŋ |
| MOTA | 1855 | | | C3007 | 12.871 | | 25.384 | 1.00 18.32 | C |
| ATOM | 1856 | | | C3007 | 12.036 | | 24.467 | 1.00 18.15 1.00 18.03 | И |
| ATOM | 1857 | NE2 | | C3007 | 12.342 | | 24.215 | 1.00 18.96 | C |
| MOTA | 1858 | С | | C3007 | 16.288 | | 25.196 | 1.00 19.65 | ō |
| ATOM | 1859 | 0 | | C3007 | 17.200 | | 24.940 | 1.00 13.03 | Ŋ |
| MOTA | 1860 | N | | C3008 | 15.795 | | 24.307 22.965 | 1.00 13.27 | C |
| ATOM | 1861 | CA | | C3008 | 16.340 | | 21.932 | 1.00 17.73 | c |
| ATOM | 1862 | С | | C3008 | 15.307 | | 22.215 | 1.00 17.73 | Ö |
| ATOM | 1863 | 0 | | C3008 | 14.398 | | 20.735 | 1.00 17.47 | N |
| MOTA | 1864 | N | | C3009 | 15.426 | | 19.658 | 1.00 18.23 | C |
| MOTA | 1865 | CA | | C3009 | 14.512 | | 19.340 | 1.00 17.95 | C |
| MOTA | 1866 | CB | | C3009 | 13.483 12.743 | | 20.604 | 1.00 17.06 | С |
| MOTA | 1867 | | | : C3009 | 14.192 | | 18.683 | 1.00 17.87 | С |
| MOTA | 1868 | | | C3009 | 13.233 | | 18.104 | 1.00 18.30 | С |
| ATOM | 1869 | | | . C3009 | 15.323 | | 18.406 | 1.00 19.18 | C |
| ATOM | 1870 | С | | C3009 | 16.51 | | 18.345 | 1.00 18.80 | 0 |
| ATOM | 1871 | O N | | C3009 | 14.682 | | 17.413 | 1.00 20.69 | N |
| ATOM | 1872 | N CA | | C3010 | 15.330 | | 16.144 | 1.00 22.71 | С |
| MOTA | 1873 1874 | CB | | C3010 | 16.25 | | 16.216 | 1.00 23.72 | С |
| MOTA | 1875 | CG | | C3010 | 16.94 | | 14.899 | 1.00 24.96 | C |
| ATOM ATOM | 1876 | | | C3010 | 17.84 | | 14.528 | 1.00 26.04 | 0 |
| ATOM | 1877 | | | C3010 | 16.59 | | 14.219 | 1.00 26.67 | 0 |
| ATOM | 1878 | C | | C3010 | 14.30 | | 15.045 | 1.00 23.50 | С |
| ATOM | 1879 | ō | | P C3010 | 13.23 | 9 24.407 | 15.278 | 1.00 23.37 | 0 |
| ATOM | 1880 | N | | E C3011 | 14.64 | 5 25.428 | 13.851 | 1.00 24.39 | N |
| ATOM | 1881 | CA | IL | E C3011 | 13.79 | 6 25.259 | 12.695 | | C |
| MOTA | 1882 | CB | | E C3011 | 13.17 | 8 26.600 | 12.239 | 1.00 25.68 | C |
| ATOM | 1883 | CG2 | 2 IL | E C3011 | 14.27 | 0 27.609 | 11.941 | | С |
| ATOM | 1884 | CG: | LIL | E C3011 | 12.27 | 4 26.364 | 11.022 | | C |
| ATOM | 1885 | CD: | | E C3011 | 11.30 | | 10.737 | 1.00 25.60 | С |
| ATOM | 1886 | С | IL | E C3011 | 14.70 | | 11.616 | | С |
| MOTA | 1887 | 0 | | E C3011 | 15.85 | | 11.476 | | 0 N |
| ATOM | 1888 | N | GL | U C3012 | 14.18 | | | 1.00 28.16 | C |
| ATOM | 1889 | CA | | U C3012 | 14.93 | | 9.829 | | C |
| MOTA | 1890 | | | U C3012 | 15.41 | | | | c |
| MOTA | 1891 | | | U C3012 | 16.34 | | | | C |
| MOTA | 1892 | | | U C3012 | 17.72 | | | | ő |
| MOTA | 1893 | | | U C3012 | 18.08 | | | | ō |
| MOTA | 1894 | | | U C3012 | 18.44 | | | | c |
| MOTA | 1895 | | | U C3012 | 14.09 | | | | ō |
| ATOM | 1896 | | | U C3012 | 12.90 | | | | N |
| MOTA | 1897 | | | U C3013 | 14.72 | | | _ | C |
| ATOM | 1898 | | | U C3013 | 14.06 | | | | c |
| ATOM | 1899 | | | U C3013 | 14.78 14.20 | | | | c |
| MOTA | 1900 |) CG | ı Gl | U C3013 | 14.2 | , | . 5.00 | . 1.00 55.05 | |
| | | | | | | | | | |

| **** | | | | | | | | | | |
|------|------|-----|------|-------|--------|--------|--------|-------|-------|---|
| ATOM | 1901 | CD | GLU | C3013 | 15.142 | 24.089 | 2.614 | 1.00 | 36.48 | С |
| ATOM | 1902 | OE1 | GLII | C3013 | 15.645 | 25.228 | 2.761 | | 36.82 | |
| | | | | | | | | | | 0 |
| ATOM | 1903 | | | C3013 | 15.376 | 23.365 | 1.622 | 1.00 | 37.39 | 0 |
| ATOM | 1904 | Ç | GLU | C3013 | 14.206 | 21.418 | 5.873 | 1.00 | 31.77 | С |
| ATOM | 1905 | 0 | GLU | C3013 | 15.306 | 20.877 | 5.914 | 1 00 | 31.08 | |
| ATOM | 1906 | N | | C3014 | | | | | | |
| | | | | | 13.093 | 20.750 | 5.614 | | 32.39 | N |
| MOTA | 1907 | CA | LEU | C3014 | 13.130 | 19.318 | 5.360 | .1.00 | 33.65 | С |
| ATOM | 1908 | CB | LEU | C3014 | 11.718 | 18.794 | 5.080 | 1.00 | 33.57 | C |
| ATOM | 1909 | CG | LEU | C3014 | 10.813 | 18.685 | 6.313 | | 34.16 | C |
| ATOM | 1910 | | | C3014 | 9.416 | 18.252 | 5.906 | | 34.65 | |
| ATOM | | | | | | | | | | C |
| | 1911 | | | C3014 | 11.404 | 17.680 | 7.280 | 1.00 | 34.38 | C |
| MOTA | 1912 | С | LEU | C3014 | 14.069 | 18.946 | 4.220 | 1.00 | 34.37 | С |
| MOTA | 1913 | 0 | LEU | C3014 | 14.736 | 17.913 | 4.271 | 1.00 | 34.47 | 0 |
| MOTA | 1914 | N | AT.A | C3015 | 14.128 | 19.801 | 3.204 | | 35.44 | N |
| ATOM | 1915 | CA | | C3015 | 14.982 | 19.572 | | | | |
| | | | | | | | 2.047 | | 36.79 | С |
| MOTA | 1916 | CB | | C3015 | 14.749 | 20.655 | 1.011 | | 36.53 | С |
| ATOM | 1917 | С | ALA | C3015 | 16.457 | 19.511 | 2.418 | 1.00 | 37.84 | С |
| ATOM | 1918 | 0 | ALA | C3015 | 17.215 | 18.737 | 1.831 | 1.00 | 38.53 | 0 |
| ATOM | 1919 | N | | C3016 | 16.863 | 20.322 | 3.391 | | 39.07 | |
| | | | | | | | | | | N |
| ATOM | 1920 | CA | | C3016 | 18.253 | 20.349 | 3.838 | | 40.09 | С |
| MOTA | 1921 | CB | SER | C3016 | 18.473 | 21.478 | 4.847 | 1.00 | 40.11 | C |
| ATOM | 1922 | OG | SER | C3016 | 18.172 | 22.734 | 4.271 | 1.00 | 41.50 | 0 |
| MOTA | 1923 | С | SER | C3016 | 18.628 | 19.026 | 4.481 | | 40.95 | c |
| ATOM | 1924 | 0 | | C3016 | 19.757 | 18.552 | | | | |
| | | | | | | | 4.340 | | 41.12 | 0 |
| ATOM | 1925 | N | | C3017 | 17.683 | 18.428 | 5.197 | 1.00 | 41.82 | N |
| MOTA | 1926 | CA | ILE | C3017 | 17.951 | 17.158 | 5.849 | 1.00 | 43.16 | С |
| ATOM | 1927 | CB | ILE | C3017 | 16.799 | 16.768 | 6.795 | 1.00 | 42.90 | С |
| ATOM | 1928 | CG2 | TLE | C3017 | 17.170 | 15.527 | 7.598 | | 42.32 | č |
| ATOM | 1929 | | | | | | | | | |
| | | | | C3017 | 16.518 | 17.924 | 7.759 | | 43.05 | С |
| ATOM | 1930 | | | C3017 | 17.709 | 18.332 | 8.597 | 1.00 | 42.53 | С |
| ATOM | 1931 | С | ILE | C3017 | 18.165 | 16.076 | 4.789 | 1.00 | 44.24 | С |
| ATOM | 1932 | 0 | ILE | C3017 | 19.033 | 15.215 | 4.941 | 1.00 | 44.09 | 0 |
| ATOM | 1933 | N | | C3018 | 17.383 | 16.128 | 3.713 | | 45.44 | |
| | | | | | | | | | | N |
| ATOM | 1934 | CA | | C3018 | 17.530 | 15.158 | 2.637 | | 47.05 | С |
| ATOM | 1935 | CB | | C3018 | 16.516 | 15.411 | 1.524 | 1.00 | 47.54 | С |
| ATOM | 1936 | CG | GĽU | C3018 | 15.158 | 14.805 | 1.755 | 1.00 | 48.25 | С |
| ATOM | 1937 | CD | GLU | C3018 | 14.383 | 14.664 | 0.463 | 1.00 | 48.87 | С |
| ATOM | 1938 | OE1 | | C3018 | 14.159 | 15.686 | -0.220 | | 49.40 | Ö |
| ATOM | 1939 | | | C3018 | | | | | | |
| | | | | | 14.005 | 13.525 | 0.126 | | 49.49 | 0 |
| MOTA | 1940 | С | | C3018 | 18.929 | 15.261 | 2.048 | 1.00 | 47.90 | С |
| ATOM | 1941 | 0 | GLU | C3018 | 19.696 | 14.299 | 2.083 | 1.00 | 47.96 | 0 |
| ATOM | 1942 | N | SER | C3019 | 19.248 | 16.429 | 1.495 | 1.00 | 48.89 | N |
| ATOM | 1943 | CA | SER | C3019 | 20.560 | 16.658 | 0.905 | | 49.72 | С |
| ATOM | 1944 | СВ | | C3019 | 20.815 | 18.152 | | | | |
| | | | | | | | 0.713 | | 49.87 | C |
| ATOM | 1945 | OG | | C3019 | 19.977 | 18.685 | -0.295 | | 50.04 | 0 |
| MOTA | 1946 | С | SER | C3019 | 21.614 | 16.078 | 1.825 | 1.00 | 50.34 | С |
| ATOM | 1947 | 0 | SER | C3019 | 22.506 | 15.362 | 1.380 | 1.00 | 50.79 | 0 |
| ATOM | 1948 | N | ALA | C3020 | 21.504 | 16:380 | 3.114 | | 50.84 | N |
| ATOM | 1949 | CA | | C3020 | 22.461 | 15.860 | 4.083 | | | |
| | | | | | | | | | 51.57 | C |
| ATOM | 1950 | CB | | C3020 | 22.054 | 16.266 | 5.491 | | 51.45 | С |
| MOTA | 1951 | С | | C3020 | 22.511 | 14.338 | 3.960 | 1.00 | 52.20 | С |
| MOTA | 1952 | 0 | ALA | C3020 | 23.585 | 13.752 | 3.811 | 1.00 | 52.03 | 0 |
| MOTA | 1953 | N | VAL | C3021 | 21.337 | 13.711 | 4.013 | | 53.10 | N |
| ATOM | 1954 | CA | | C3021 | 21.212 | 12.259 | 3.897 | | | |
| ATOM | | | | C3021 | | | | | 53.96 | C |
| | 1955 | CB | | | 19.730 | 11.818 | 3.969 | | 53.97 | С |
| MOTA | 1956 | | | C3021 | 19.609 | 10.329 | 3.671 | 1.00 | 54.14 | C |
| ATOM | 1957 | CG2 | VAL | C3021 | 19.165 | 12.124 | 5.340 | 1.00 | 53.98 | C |

| ATOM | 1958 | С | VAL | C3021 | 21.788 | 11.793 | 2.566 | 1.00 54.57 | С |
|--------------|--------------|---------|-----|----------------|------------------|------------------|----------------|--------------------------|--------|
| MOTA | 1959 | 0 | VAL | C3021 | 22.424 | 10.740 | 2.481 | 1.00 54.43 | Ō |
| MOTA | 1960 | N | THR | C3022 | 21.553 | 12.591 | 1.530 | 1.00 55.21 | N |
| MOTA | 1961 | CA | THR | C3022 | 22.041 | 12.293 | 0.194 | 1.00 55.84 | С |
| MOTA | 1962 | CB | THR | C3022 | 21.456 | 13.283 | -0.831 | 1.00 55.80 | C |
| ATOM | 1963 | OG1 | THR | C3022 | 20.034 | 13.124 | -0.878 | 1.00 55.98 | 0 |
| MOTA | 1964 | CG2 | THR | C3022 | 22.036 | 13.036 | -2.214 | 1.00 55.79 | С |
| MOTA | 1965 | С | THR | C3022 | 23.566 | 12.355 | 0.155 | 1.00 56.35 | С |
| MOTA | 1966 | 0 | THR | C3022 | 24.213 | 11.386 | -0.230 | 1.00 56.58 | 0 |
| ATOM | 1967 | N | ARG | C3023 | 24.135 | 13.489 | 0.557 | 1.00 56.81 | N |
| ATOM | 1968 | CA | ARG | C3023 | 25.586 | 13.650 | 0.567 | 1.00 57.20 | С |
| MOTA | 1969 | CB | ARG | C3023 | 25.966 | 15.015 | 1.151 | 1.00 57.25 | С |
| MOTA | 1970 | CG | | C3023 | 27.463 | 15.289 | 1.151 | 1.00 57.60 | С |
| MOTA | 1971 | CD | ARG | C3023 | 27.782 | 16.762 | 1.388 | 1.00 57.64 | С |
| MOTA | 1972 | NE | ARG | C3023 | 27.410 | 17.222 | 2.722 | 0.05 57.76 | N |
| MOTA | 1973 | CZ | ARG | C3023 | 27.609 | 18.460 | 3.163 | 0.05 57.81 | C |
| MOTA | 1974 | | | C3023 | 28.176 | 19.364 | 2.374 | 0.05 57.84 | N |
| ATOM | 1975 | NH2 | ARG | C3023 | 27.245 | 18.796 | 4.393 | 0.05 57.82 | N |
| ATOM | 1976 | С | | C3023 | 26.203 | 12.522 | 1.390 | 1.00 57.47 | С |
| ATOM | 1977 | 0 | | C3023 | 26.328 | 11.402 | 0.903 | 1.00 57.73 | 0 |
| ATOM | 1978 | N | | C3024 | 26.592 | 12.806 | 2.630 | 1.00 57.66 | И |
| ATOM | 1979 | CA | | C3024 | 27.168 | 11.773 | 3.486 | 1.00 57.79 | С |
| MOTA | 1980 | CB | | C3024 | 27.968 | 12.404 | 4.627 | 0.05 57.91 | С |
| ATOM | 1981 | CG | | C3024 | J29.442 | 12.449 | 4.375 | 0.05 58.00 | С |
| ATOM | 1982 | | | C3024 | 30.301 | 13.491 | 4.278 | 0.05 58.04 | С |
| ATOM | 1983 | | | C3024 | 30.198 | 11.312 | 4.187 | 0.05 58.04 | N |
| ATOM | 1984 | | | C3024 | 31.459 | 11.651 | 3.986 | 0.05 58.06 | С |
| ATOM | 1985 | | | C3024 | . 31.549 | 12.968 | 4.036 | 0.05 58.07 | N |
| ATOM | 1986 | С | | C3024 | 26.069 | 10.873 | 4.054 | 1.00 57.96 | С |
| ATOM | 1987 | 0 | | C3024 | 25.413 | 11.223 | 5.038 | 1.00 58.10 | 0 |
| ATOM | 1988 | N | | C3025 | 25.874 | 9.710 | 3.435 | 1.00 57.92 | N |
| ATOM | 1989 | CA | | C3025 | 24.846 | 8.773 | 3.879 | 1.00 57.71 | · |
| ATOM | 1990 | CB | | C3025 | 24.824 | 7.535 | 2.976 | 1.00 58.27 | С |
| ATOM | 1991 | CG | | C3025 | 25.979 | 6.571 | 3.189 | 1.00 59.11 | С |
| ATOM | 1992 | CD | | C3025 | 25.784 | 5.259 | 2.446 | 1.00 59.59 | C |
| ATOM | 1993 | | | C3025 | 24.749 | 4.592 | 2.673 | 1.00 59.65 | 0 |
| ATOM | 1994 | OE2 | | C3025 | 26.665 | 4.893 | 1.637 | 1.00 59.98 | 0 |
| ATOM | 1995 | C | | C3025 | 25.029 | 8.341 | 5.336 | 1.00 57.11 | C |
| ATOM | 1996 | 0 | | C3025 | 24.089 | 7.857 | 5.974 | 1.00 57.33 | 0 |
| ATOM | 1997 | N | | C3026 | 26.238 | 8.508 | 5.861 | 1.00 56.15 | N |
| ATOM | 1998 | CA | | C3026 | 26.486 | 8.136 | 7.242 | 1.00 55.03 | C |
| ATOM | 1999 | C | | C3026 | 25.890 | 9.170 | 8.177 | 1.00 54.19 | C |
| ATOM | 2000 | 0 | | C3026 | 26.023 | 9.081 | 9.398 | 1.00 54.12 | 0 |
| ATOM | 2001 | N C2 | | C3027 | 25.227 | 10.160 | 7.589 | 1.00 53.18 | N |
| ATOM | 2002 2003 | CA | | C3027 | 24.601 | 11.238 | 8.343 | 1.00 52.05 | C |
| MOTA | | CB | | | 23.817 | 12.142 | 7.386 | 1.00 52.10 | C |
| ATOM | 2004 | CG | | C3027 | 23.129 | 13.289 | 8.059 | 1.00 52.03 | C |
| MOTA MOTA | 2005 2006 | | | C3027 | 23.859 21.743 | 14:233 | 8.768 | 1.00 51.96 | C |
| ATOM | 2007 | | | C3027 C3027 | | 13.427 | 7.984 | 1.00 52.34 1.00 52.41 | C |
| ATOM | 2007 | | | | 23.221 | 15.304 | 9.398 | | С |
| ATOM | 2008 | CZ | | C3027 | 21.092 | 14.492 | 8.609 9.319 | 1.00 52.33 1.00 52.40 | c c |
| ATOM | 2010 | C | | C3027 | 23.676 | 15.434 10.720 | 9.443 | 1.00 52.40 | |
| ATOM | 2010 | 0 | | C3027 | 23.914 | 10.720 | 10.628 | 1.00 51.01 | C 0 |
| ATOM | 2012 | Ŋ | | C3028 | 22.631 | 10.002 | 9.042 | 1.00 31.01 | N |
| ATOM | 2013 | CA | | C3028 | 21.648 | 9.463 | 9.979 | 1.00 49.81 | C |
| ATOM | 2014 | CB | | C3028 | 20.608 | 8.645 | 9.231 | 1.00 48.74 | c |
| | | ~~ | 1 | | 20.000 | 0.013 | J. 2JI | | C |

| ATOM | 2015 | С | ALA | C3028 | 22.240 | 8.630 | 11.104 | 1.00 48.04 | С |
|------|------|-----|-----|--------|--------|--------|--------|------------|---|
| ATOM | 2016 | 0 | ALA | C3028 | 21.865 | 8.802 | 12.266 | 1.00 47.95 | 0 |
| ATOM | 2017 | N | LYS | C3029 | 23.156 | 7.726 | 10.767 | 1.00 47.14 | N |
| ATOM | 2018 | CA | LYS | C3029 | 23.765 | 6.874 | 11.779 | 1.00 46.13 | C |
| ATOM | 2019 | CB | LYS | C3029 | 24.681 | 5.833 | 11.126 | 1.00 46.10 | C |
| ATOM | 2020 | CG | LYS | C3029 | 25.918 | 6.410 | 10.460 | 0.05 46.12 | С |
| ATOM | 2021 | CD | LYS | C3029 | 26.810 | 5.310 | 9.907 | 0.05 46.11 | C |
| ATOM | 2022 | CE | LYS | C3029 | 28.065 | 5.884 | 9.269 | 0.05 46.11 | C |
| ATOM | 2023 | NZ | LYS | C3029 | 28.873 | 6.675 | 10.238 | 0.05 46.11 | N |
| ATOM | 2024 | С | LYS | C3029 | 24.548 | 7.709 | 12.789 | 1.00 45.54 | С |
| ATOM | 2025 | 0 | LYS | C3029 | 24.739 | 7.299 | 13.936 | 1.00 45.54 | 0 |
| ATOM | 2026 | N | ARG | C3030 | 24.997 | 8.883 | 12.361 | 1.00 44.50 | N |
| ATOM | 2027 | CA | ARG | C3030 | 25.747 | 9.770 | 13.243 | 1.00 43.62 | С |
| ATOM | 2028 | СB | ARG | C3030 | 26.703 | 10.650 | 12.425 | 1.00 43.71 | C |
| ATOM | 2029 | CG | ARG | C3030 | 28.071 | 10.019 | 12.194 | 0.05 43.64 | С |
| ATOM | 2030 | CD | ARG | C3030 | 28.410 | 9.914 | 10.717 | 0.05 43.63 | С |
| MOTA | 2031 | NE | ARG | C3030- | 28.407 | 11.214 | 10.051 | 0.05 43.58 | N |
| ATOM | 2032 | CZ | ARG | C3030 | 28.653 | 11.389 | 8.756 | 0.05 43.55 | C |
| MOTA | 2033 | NH1 | ARG | C3030 | 28.923 | 10.347 | 7.983 | 0.05 43.53 | N |
| MOTA | 2034 | NH2 | ARG | C3030 | 28.626 | 12.608 | 8.234 | 0.05 43.55 | N |
| ATOM | 2035 | С | ARG | C3030 | 24.819 | 10.651 | 14.071 | 1.00 42.89 | C |
| ATOM | 2036 | 0 | | C3030 | 25.183 | 11.099 | 15.158 | 1.00 42.93 | 0 |
| ATOM | 2037 | N | VAL | C3031 | 23.616 | 10.885 | 13.556 | 1.00 41.77 | N |
| ATOM | 2038 | CA | VAL | C3031 | 22.637 | 11.724 | 14.237 | 1.00 40.54 | С |
| ATOM | 2039 | CB | | C3031 | 21.761 | 12.464 | 13.213 | 1.00 40.55 | С |
| ATOM | 2040 | | | C3031 | 20.717 | 13.298 | 13.926 | 1.00 40.68 | С |
| ATOM | 2041 | | | C3031 | 22.631 | 13.339 | 12.328 | 1.00 40.57 | С |
| ATOM | 2042 | С | VAL | C3031 | 21.727 | 10.941 | 15.180 | 1.00 39.76 | С |
| ATOM | 2043 | 0 | VAL | C3031 | 21.373 | 11.418 | 16.256 | 1.00 39.22 | 0 |
| ATOM | 2044 | N | | C3032 | 21.353 | 9.736 | 14.771 | 1.00 39.10 | N |
| ATOM | 2045 | CA | LEU | C3032 | 20.470 | 8.905 | 15.572 | 1.00 38.53 | С |
| ATOM | 2046 | CB | LEU | C3032 | 19.453 | 8.223 | 14.656 | 1.00 38.36 | С |
| ATOM | 2047 | CG | LEU | C3032 | 18.612 | 9.150 | 13.767 | 1.00 38.42 | C |
| ATOM | 2048 | CD1 | LEU | C3032 | 17.671 | 8.308 | 12.912 | 1.00 38.50 | С |
| ATOM | 2049 | CD2 | LEU | C3032 | 17.819 | 10.131 | 14.622 | 1.00 37.90 | С |
| ATOM | 2050 | С | LEU | C3032 | 21.217 | 7.848 | 16.378 | 1.00 38.18 | С |
| ATOM | 2051 | 0 | LEU | C3032 | 22.395 | 7.585 | 16.134 | 1.00 38.41 | 0 |
| ATOM | 2052 | N | THR | C3033 | 20.530 | 7.263 | 17.356 | 1.00 37.76 | N |
| ATOM | 2053 | CA | THR | C3033 | 21.105 | 6.193 | 18.166 | 1.00 37.32 | С |
| MOTA | 2054 | CB | THR | C3033 | 20.636 | 6.248 | 19.638 | 1.00 37.17 | C |
| MOTA | 2055 | OG1 | THR | C3033 | 19.233 | 5.967 | 19.704 | 1.00 37.15 | 0 |
| ATOM | 2056 | CG2 | THR | C3033 | 20.900 | 7.612 | 20.236 | 1.00 37.54 | С |
| ATOM | 2057 | С | THR | C3033 | 20.546 | 4.918 | 17.537 | 1.00 37.05 | С |
| ATOM | 2058 | 0 | THR | C3033 | 19.725 | 4.992 | 16.623 | 1.00 36.86 | 0 |
| ATOM | 2059 | N | ALA | C3034 | 20.976 | 3.759 | 18.026 | 1.00 37.00 | N |
| ATOM | 2060 | CA | ALA | C3034 | 20.502 | 2.481 | 17.495 | 1.00 36.98 | С |
| ATOM | 2061 | CB | ALA | C3034 | 21.121 | -1.324 | 18.279 | 1.00 36.85 | С |
| ATOM | 2062 | С | ALA | C3034 | 18.978 | 2.384 | 17.538 | 1.00 36.93 | С |
| ATOM | 2063 | 0 | | C3034 | 18.331 | 2.154 | 16.516 | 1.00 36.95 | 0 |
| MOTA | 2064 | N | | C3035 | 18.401 | 2.553 | 18.721 | 1.00 37.04 | N |
| MOTA | 2065 | CA | | C3035 | 16.951 | 2.480 | 18.844 | 1.00 37.28 | С |
| ATOM | 2066 | CB | | C3035 | 16.522 | 2.844 | 20.271 | 1.00 37.10 | C |
| MOTA | 2067 | CG | | C3035 | 15.183 | 2.291 | 20.770 | 0.05 37.08 | C |
| ATOM | 2068 | | | C3035 | 14.994 | 2.675 | 22.229 | 0.05 37.00 | C |
| ATOM | 2069 | CD2 | | C3035 | 14.040 | 2.822 | 19.922 | 0.05 37.02 | С |
| MOTA | 2070 | С | | C3035 | 16.322 | 3.442 | 17.828 | 1.00 37.52 | C |
| MOTA | 2071 | 0 | LEU | C3035 | 15.418 | 3.065 | 17.084 | 1.00 37.65 | 0 |
| | | | | | | | | | |

| ATOM | 2072 | N | GLU | C3036 | 16.81 | 4 4.678 | 17.790 | 1.00 37 | 7.89 | | Ν . |
|------|------|-----|-----|---------|-------|------------|--------|---------|-------|---|-----|
| ATOM | 2073 | CA | GLU | C3036 | 16.29 | 9 5.679 | 16.854 | 1.00 38 | 3.14 | | С |
| ATOM | 2074 | СВ | GLU | C3036 | 17.00 | 7.031 | 17.063 | 1.00 37 | 7.82 | | С |
| ATOM | 2075 | CG | GLU | C3036 | 16.48 | 6 7.857 | 18.244 | 1.00 37 | 7.71 | | С |
| ATOM | 2076 | CD | GLU | C3036 | 17.30 | 5 9.128 | 18.490 | 1.00 37 | | | С |
| ATOM | 2077 | OE1 | GLU | C3036 | 16.86 | 5 9.989 | 19.283 | 1.00 37 | 7.10 | | 0 |
| ATOM | 2078 | OE2 | GLU | C3036 | 18.39 | 7 9.265 | 17.896 | 1.00 37 | 7.62 | | 0 |
| ATOM | 2079 | С | | C3036 | 16.46 | 2 5.232 | 15.398 | 1.00 38 | 3.18 | | С |
| ATOM | 2080 | 0 | GLU | C3036 | 15.62 | 9 5.551 | 14.553 | 1.00 38 | 3.25 | | 0 |
| ATOM | 2081 | N | MET | C3037 | 17.53 | | 15.104 | 1.00 38 | 3.56 | | N |
| ATOM | 2082 | CA | | C3037 | 17.76 | 9 4.022 | 13.743 | 1.00 39 | 9.53 | | С |
| ATOM | 2083 | СВ | | C3037 | 19.19 | 6 3.495 | 13.591 | 1.00 40 | 0.21 | | С |
| ATOM | 2084 | CG | MET | C3037 | 20.23 | 0 4.576 | 13.312 | 1.00 43 | 1.61 | | С |
| ATOM | 2085 | SD | | C3037 | 19.93 | | 11.726 | 1.00 43 | 3.58 | | S |
| ATOM | 2086 | CE | | C3037 | 20.79 | | 10.578 | 1.00 43 | 2.57 | | С |
| ATOM | 2087 | C | | C3037 | 16.78 | | 13.337 | 1.00 3 | 9.68 | | С |
| ATOM | 2088 | 0 | | C3037 | 16.35 | | 12.186 | 1.00 3 | 9.73 | | 0 |
| ATOM | 2089 | N | | C3038 | 16.42 | | 14.284 | 1.00 3 | 9.82 | | N |
| ATOM | 2090 | CA | | C3038 | 15.47 | | 14.012 | 1.00 3 | 9.88 | | С |
| ATOM | 2091 | CB | | C3038 | 15.20 | | 15.289 | 1.00 3 | 9.75 | | С |
| ATOM | 2092 | CG | | C3038 | 16.45 | | 15.905 | 0.05 3 | | | С |
| ATOM | 2093 | CD | | C3038 | 16.16 | | 17.213 | 0.05 3 | 9.67 | | С |
| ATOM | 2094 | | | C3038 | 15.34 | | 17.210 | 0.05 3 | 9.64 | | 0 |
| ATOM | 2095 | | | C3038 | 16.75 | | 18.243 | 0.05 3 | 9.61 | | 0 |
| ATOM | 2096 | C | | C3038 | 14.17 | | 13.500 | 1.00 4 | 0.09 | | C |
| ATOM | 2097 | o | | C3038 | 13.55 | | 12.559 | 1.00 4 | 0.19 | | 0 |
| ATOM | 2098 | N | | C3039 | 13.77 | | 14.126 | 1.00 4 | | | N |
| ATOM | 2099 | CA | | C3039 | 12.56 | | 13.744 | 1.00 4 | 0.26 | | С |
| ATOM | 2100 | CB | | C3039 | 12.23 | | 14.811 | 1.00 4 | 0.88 | | С |
| ATOM | 2101 | CG | | C3039 | 11.10 | | 14.468 | 1.00 4 | | | С |
| ATOM | 2102 | CD | | C3039 | 9.75 | | 14.377 | 1.00 4 | | | С |
| ATOM | 2102 | NE | | C3039 | 8.6 | | 14.425 | 1.00 4 | | | N |
| ATOM | 2103 | CZ | | C3039 | 7.39 | | 14.169 | 1.00 4 | | | С |
| MOTA | 2105 | | | C3039 | 7.00 | | 13.838 | 1.00 4 | | | N |
| ATOM | 2106 | | | C3039 | 6.49 | | 14.234 | 1.00 4 | 4.15 | | N |
| ATOM | 2107 | C | | C3039 | 12.79 | | 12.384 | 1.00 3 | | | С |
| ATOM | 2108 | Ö | | C3039 | 11.89 | | 11.506 | 1.00 3 | 9.45 | | 0 |
| ATOM | 2109 | N | | C3040 | 13.90 | | 12.216 | 1.00 4 | 0.04 | • | N |
| ATOM | 2110 | CA | | C3040 | 14.2 | | 10.968 | 1.00 4 | 0.26 | | С |
| ATOM | 2111 | CB | | C3040 | 15.60 | 03 6.074 | 11.061 | 1.00 4 | 0.27 | | C |
| ATOM | 2112 | CG | | C3040 | 16.0 | 22 6.804 | 9.814 | 1.00 4 | 0.95 | | С |
| ATOM | 2113 | | PHE | C3040 | 15.4 | 31 8.015 | 9.466 | 1.00 4 | 1.11 | | С |
| ATOM | 2114 | CD2 | PHE | C3040 | 17.0 | 13 6.282 | 8.989 | 1.00 4 | 1.10 | | С |
| ATOM | 2115 | CE1 | PHE | C3040 | 15.8 | 22 8.699 | 8.315 | 1.00 4 | 11.43 | | С |
| MOTA | 2116 | CE2 | PHE | C3040 | 17.4 | 12 6.956 | 7.835 | 1.00 4 | 11.44 | | С |
| ATOM | 2117 | CZ | | C3040 | 16.8 | 15 8.169 | 7.497 | 1.00 4 | | | С |
| ATOM | 2118 | C | PHE | C3040 | 14.1 | 81 - 4.507 | 9.756 | 1.00 4 | 10.43 | | С |
| ATOM | 2119 | 0 | PHE | C3040 | 13.4 | 67 4:757 | 8.784 | 1.00 3 | 39.60 | | 0 |
| ATOM | 2120 | N | THE | R C3041 | 14.9 | 56 3.429 | 9.833 | 1.00 4 | 10.82 | | N |
| ATOM | 2121 | CA | THE | R C3041 | 15.0 | 43 2.459 | | 1.00 4 | | | С |
| ATOM | 2122 | СВ | | R C3041 | 16.1 | 54 1.435 | | 1.00 4 | | | С |
| ATOM | 2123 | OG1 | THE | R C3041 | 15.7 | 82 0.597 | | 1.00 4 | | | 0 |
| ATOM | 2124 | | | R C3041 | 17.4 | 50 2.149 | 9.351 | 1.00 4 | | | С |
| ATOM | 2125 | С | THI | R C3041 | 13.7 | | | | | | С |
| MOTA | 2126 | 0 | THI | R C3041 | 13.6 | | | • | | | 0 |
| MOTA | 2127 | N | SEI | R C3042 | 12.7 | | | | | | N |
| ATOM | 2128 | CA | SE | R C3042 | 11.5 | 21 1.059 | 9.152 | 1.00 | 41.35 | | С |

| ATOM | 2129 | CB | SER | C3042 | 10.998 | 0.445 | 10.454 | 1.00 41.25 | С |
|--------------|--------------|----------|-------|----------------|------------------|------------------|----------------|--------------------------|--------|
| ATOM | 2130 | OG | SER | C3042 | 10.501 | 1.442 | 11.324 | 1.00 42.03 | 0 |
| ATOM | 2131 | С | SER | C3042 | 10.469 | 1.996 | 8.569 | 1.00 41.30 | С |
| ATOM | 2132 | 0 | SER | C3042 | 9.334 | 1.589 | 8.311 | 1.00 41.45 | 0 |
| ATOM | 2133 | | | C3043 | 10.850 | 3.255 | 8.373 | 1.00-41.13 | N |
| MOTA | 2134 | | | C3043 | 9.956 | 4.262 | 7.808 | 1.00 40.94 | C |
| ATOM | 2135 | CB | | C3043 | 10.026 | 5.566 | 8.618 | 1.00 40.70 | C |
| ATOM | 2136 | CG | | C3043 | 9.382 | 5.618 | 10.012 | 1.00 40.56 | С |
| MOTA | 2137 | | | C3043 | .9.835 | 6.871 | 10.735 | 1.00 40.07 | C |
| MOTA | 2138 | | | C3043 | 7.859 | 5.586 | 9.891 | 1.00 40.06 | . C |
| MOTA | 2139 | С | | C3043 | 10.398 | 4.528 | 6.375 | 1.00 41.07 1.00 40.93 | 0 |
| MOTA | 2140 | 0 | | C3043 | 11.494 | 4.128 | 5.978 | 1.00 40.93 | N |
| ATOM | 2141 | N | | C3044 | 9.550 | 5.203 5.513 | 5.604 4.214 | 1.00 41.20 | C |
| ATOM | 2142 | CA | | C3044 | 9.871 9.481 | 4.346 | 3.307 | 1.00 42.49 | Ċ |
| ATOM | 2143 | CB | | C3044 C3044 | 7.982 | 4.199 | 3.107 | 1.00 43.64 | c |
| ATOM | 2144 | CG | | C3044 | 7.678 | 3.191 | 2.012 | 1.00 45.17 | C |
| ATOM | 2145 | CE | | C3044 | 6.206 | 3.228 | 1.616 | 1.00 45.99 | C |
| ATOM ATOM | 2146 2147 | NZ | | C3044 | 5.900 | 2.249 | 0.535 | 1.00 47.05 | N |
| ATOM | 2148 | C | | C3044 | 9.147 | 6.768 | 3.739 | 1.00 40.92 | С |
| ATOM | 2149 | Ö | | C3044 | 8.191 | 7.219 | 4.365 | 1.00 40.90 | 0 |
| ATOM | 2150 | N | | C3045 | 9.605 | 7.320 | 2.621 | 1.00 40.22 | N |
| ATOM | 2151 | CA | | C3045 | 8.986 | 8.510 | 2.072 | 1.00 39.26 | С |
| ATOM | 2152 | C | | C3045 | 9.182 | 9.736 | 2.937 | 1.00 38.68 | С |
| ATOM | 2153 | 0 | GLY | C3045 | 10.142 | 9.829 | 3.694 | 1.00 38.24 | 0 |
| ATOM | 2154 | N | ARG | C3046 | 8.260 | 10.683 | 2.818 | 1.00 38.56 | N |
| MOTA | 2155 | CA | ARG | C3046 | 8.318 | 11.921 | 3.589 | 1.00 38.49 | С |
| ATOM | 2156 | CB | ARG | C3046 | 7.107 | 12.793 | 3.251 | 1.00 38.44 | С |
| ATOM | 2157 | CG | ARG | C3046 | 7.104 | 14.158 | 3.912 | 0.05 38.46 | C |
| ATOM | 2158 | CD | ARG | C3046 | 5.887 | 14.963 | 3.483 | 0.05 38.40 | C |
| MOTA | 2159 | NE | ARG | C3046 | 5.874 | 15.200 | 2.042 | 0.05 38.36 | N |
| MOTA | 2160 | CZ | | C3046 | 4.887 | 15.809 | 1.393 | 0.05 38.32 | C |
| MOTA | 2161 | | | C3046 | 4.963 | 15.982 | 0.081 | 0.05 38.29 | N N |
| MOTA | 2162 | | | C3046 | 3.822 | 16.241 | 2.055 | 0.05 38.31 1.00 38.25 | C |
| ATOM | 2163 | С | | C3046 | 8.372 | 11.647 | 5.093 5.830 | 1.00 38.23 | Ö |
| ATOM | 2164 | 0 | | C3046 | 9.027 | 12.365 10.595 | 5.538 | 1.00 38.32 | N |
| ATOM | 2165 | N | | C3047 C3047 | 7.696 7.673 | 10.234 | 6.953 | 1.00 38.52 | C |
| ATOM | 2166 2167 | CA CB | | C3047 | 6.727 | 9.051 | 7.169 | 1.00 39.67 | C |
| ATOM ATOM | 2168 | CG | | C3047 | 5.251 | 9.432 | 7.225 | 1.00 41.67 | С |
| ATOM | 2169 | CD | | C3047 | 4.369 | 8.277 | 6.767 | 1.00 43.70 | С |
| ATOM | 2170 | NE | | C3047 | 3.141 | 8.152 | 7.550 | 1.00 45.24 | N |
| ATOM | 2171 | CZ | | C3047 | 3.112 | 7.824 | 8.840 | 1.00 46.12 | С |
| ATOM | 2172 | | | C3047 | 4.248 | 7.589 | 9.495 | 1.00 46.08 | N |
| ATOM | 2173 | | | C3047 | 1.947 | 7.722 | 9.474 | 1.00 45.94 | N |
| MOTA | 2174 | С | ARG | C3047 | 9.042 | 9.906 | 7.554 | 1.00 38.04 | C |
| ATOM | 2175 | 0 | ARG | C3047 | 9.287 | -10.174 | 8.731 | 1.00 37.75 | 0 |
| MOTA | 2176 | N | | C3048 | 9.931 | 9.320 | 6.757 | 1.00 37.49 | N |
| MOTA | 2177 | CA | | C3048 | 11.258 | 8.966 | | 1.00 36.91 | C |
| ATOM | 2178 | CB | | C3048 | 11.912 | 7.919 | | 1.00 36.94 | C |
| MOTA | 2179 | ÇG | | C3048 | 13.283 | 7.496 | | 1.00 37.10 1.00 37.40 | C |
| ATOM | 2180 | CD | | C3048 | 14.092 | 6.744 | | 1.00 37.40 | 0 |
| ATOM | 2181 | | | C3048 | 14.233 | 7.196 5.600 | | 1.00 37.42 | N |
| ATOM | 2182 | | | C3048 | 14.643 12.186 | 10.176 | | 1.00 37.18 | C |
| MOTA MOTA | 2183 2184 | C O | | C3048 | 12.180 | 10.284 | | 1.00 36.44 | ō |
| ATOM | 2184 | N | | C3048 | 12.101 | 11.082 | | 1.00 35.91 | N |
| U TOU | 2100 | 1.4 | - 111 | . 05045 | 12.101 | | | | |

| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | ATOM | 2186 | CA | TIF. | C3049 | | 12.932 | 12.271 | 6.429 | 1.00 35 | .80 | С |
|--|------|------|-----|------|---------|---|--------|--------|--------|---------|-------|-----|
| NEON 2188 | | | | | | • | | | 5.054 | 1.00 36 | .41 | С |
| ATOM 2189 CC1 ILE C3049 13.678 14.307 5.136 1.00 36.64 C ATOM 2190 CD1 ILE C3049 15.150 14.108 5.433 1.00 37.22 C ATOM 2191 C ILE C3049 12.436 13.201 7.542 1.00 35.41 C ATOM 2192 O ILE C3049 13.231 13.824 8.254 1.00 35.47 O ATOM 2193 N GLU C3050 11.119 13.280 7.707 1.00 34.48 N ATOM 2194 CA GLU C3050 0.546 14.118 8.756 1.00 33.55 C C C C C C C C C | | | | | | | | | 4.607 | 1.00 37 | .11 | С |
| ATOM 2190 CDI ILE C3049 15.150 14.108 5.433 1.00 37.22 C C ATOM 2191 C ILE C3049 13.201 7.542 1.00 35.41 C ATOM 2193 N GLU C3050 11.119 13.201 7.072 1.00 35.41 N ATOM 2193 N GLU C3050 11.119 13.201 7.072 1.00 35.47 N ATOM 2193 N GLU C3050 11.119 13.280 7.707 1.00 36.48 N ATOM 2195 CB GLU C3050 9.023 14.074 8.699 1.00 34.48 C ATOM 2195 CB GLU C3050 9.023 14.074 8.699 1.00 33.55 C ATOM 2197 CD GLU C3050 8.671 14.609 7.410 1.00 36.22 C ATOM 2197 CD GLU C3050 8.671 14.609 7.410 1.00 36.22 C ATOM 2197 CD GLU C3050 6.543 13.291 7.807 1.00 37.41 C ATOM 2199 OEZ GLU C3050 6.543 13.291 7.807 1.00 37.41 C ATOM 2199 OEZ GLU C3050 6.543 13.291 7.807 1.00 37.87 O ATOM 2199 OEZ GLU C3050 6.543 13.291 7.807 1.00 37.87 O ATOM 2020 C GLU C3050 11.018 13.620 10.16 1.00 37.87 O ATOM 2020 C GLU C3050 11.018 13.620 10.16 1.00 37.87 O ATOM 2020 C GLU C3050 11.018 13.620 10.16 1.00 37.87 O ATOM 2020 C GLU C3050 11.275 14.412 11.023 1.00 31.96 O ATOM 2020 C T TYR C3051 11.130 12.303 10.251 1.00 30.44 N ATOM 2020 C GLU C3050 11.275 14.412 11.023 1.00 31.96 O ATOM 2020 C T TYR C3051 11.438 10.191 11.433 1.00 29.38 C ATOM 2020 C GLU C3050 11.438 10.191 11.433 1.00 29.38 C ATOM 2020 C GLU TYR C3051 11.438 10.191 11.433 1.00 29.38 C ATOM 2020 C C TYR C3051 11.393 8.864 12.675 1.00 27.96 C ATOM 2020 C C TYR C3051 11.593 8.896 12.741 1.00 27.15 C ATOM 2020 C C TYR C3051 11.593 8.896 12.741 1.00 27.15 C ATOM 2020 C C TYR C3051 11.593 8.896 12.914 1.00 27.15 C ATOM 2020 C C TYR C3051 11.593 8.896 12.914 1.00 27.15 C ATOM 2020 C C TYR C3051 11.593 8.896 12.914 1.00 27.15 C ATOM 2021 C C TYR C3051 13.344 7.735 16.187 1.00 27.13 C ATOM 2021 C C TYR C3051 13.347 7.73 1.00 27.10 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.10 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.10 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.70 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.70 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.70 C C ATOM 2021 C C TYR C3051 13.349 12.117 11.818 1.00 27.70 C C ATOM 2021 C | | | | | | | | | | 1.00 36 | .64 | С |
| ATOM 2191 C ILE C3049 13.231 13.824 8.254 1.00 35.41 C ATOM 2192 O ILE C3049 13.231 13.824 8.254 1.00 35.47 O ATOM 2193 N GLU C3050 11.119 13.280 7.707 1.00 34.48 N ATOM 2194 CA GLU C3050 10.546 14.118 8.756 1.00 34.18 C ATOM 2195 CB GUU C3050 8.471 14.609 7.410 1.00 34.18 C ATOM 2196 CG GLU C3050 8.471 14.609 7.410 1.00 36.22 C ATOM 2197 CD GLU C3050 6.318 15.078 6.591 1.00 37.41 C ATOM 2199 OEZ GLU C3050 6.318 15.078 6.531 1.00 37.41 C ATOM 2199 OEZ GLU C3050 6.318 15.078 6.531 1.00 37.87 O ATOM 2199 OEZ GLU C3050 6.318 15.078 6.531 1.00 37.87 O ATOM 2200 C GLU C3050 11.275 14.412 11.003 10.253 O ATOM 2201 O GLU C3050 11.275 14.412 11.003 10.253 O C ATOM 2201 C GLU C3050 11.275 14.412 11.003 10.253 O C ATOM 2201 C GLU C3050 11.275 14.412 11.003 10.00 35.44 N ATOM 2202 N TYR C3051 11.574 11.715 11.501 1.00 30.44 N ATOM 2202 C G TYR C3051 11.388 10.191 11.433 1.00 28.33 C ATOM 2204 CB TYR C3051 11.388 10.191 11.433 1.00 28.33 C ATOM 2205 CG TYR C3051 11.388 10.191 11.433 1.00 28.33 C ATOM 2205 CG TYR C3051 11.396 9.478 12.675 1.00 27.96 C ATOM 2207 CEI TYR C3051 13.334 8.964 12.741 1.00 27.15 C ATOM 2208 CD TYR C3051 13.334 8.964 12.741 1.00 27.15 C ATOM 2209 CEZ TYR C3051 13.334 8.964 12.741 1.00 27.15 C ATOM 2209 CEZ TYR C3051 13.334 8.964 12.741 1.00 27.15 C ATOM 2209 CEZ TYR C3051 13.344 7.735 16.187 1.00 27.13 C ATOM 2210 C TYR C3051 13.344 7.735 16.187 1.00 27.10 C ATOM 2211 O H TYR C3051 13.344 7.735 16.187 1.00 27.00 C ATOM 2211 O H TYR C3051 13.344 7.735 16.187 1.00 27.00 C ATOM 2212 C TYR C3051 13.344 7.735 16.187 1.00 27.00 C ATOM 2213 C TYR C3051 13.344 7.735 16.187 1.00 27.17 C C ATOM 2214 N LEU C3052 13.806 12.065 8.29 9.761 1.00 27.77 C C ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.05 C C ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.05 C C ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.06 C C ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.06 C C ATOM 2215 CA LEU C3052 16.156 14.309 11.211 1.00 27.76 C C ATOM 2226 CA ALA C3053 14.743 11.925 12.599 1.10 1.00 26.677 N ATOM 2 | | | | | | | | | 5.433 | 1.00 37 | .22 | С |
| ATOM 2192 0 ILE C3049 13.231 13.824 8.254 1.00 35.47 0 ATOM 2193 N GLU C3050 11.119 13.280 7.707 1.00 34.48 N ATOM 2195 CB GLU C3050 9.023 14.074 8.699 1.00 34.18 CA GLU C3050 8.471 14.609 7.410 1.00 36.22 CA GLU C3050 6.543 13.291 7.807 1.41 0.00 36.22 CA GLU C3050 6.543 13.291 7.807 1.41 0.00 37.41 CA GLU C3050 6.543 13.291 7.807 1.00 38.55 OATOM 2199 0E2 GLU C3050 11.018 13.620 10.116 1.00 32.30 CA GLU C3050 11.130 12.303 10.251 1.00 33.44 N GLU C3050 11.374 11.715 11.501 1.00 22.38 CA GLU C3050 11.374 11.715 11.501 1.00 22.38 CA GLU C3050 11.334 10.191 11.433 1.00 28.33 CA GLU C3050 CA TYR C3051 13.324 8.964 12.741 1.00 27.15 CA GLU C3050 13.324 8.964 12.741 1.00 27.15 CA GLU C3050 13.344 7.735 16.187 1.00 27.96 CA GLU C3050 12.895 8.290 15.014 1.00 27.13 CA GLU C3050 13.344 7.735 16.187 1.00 27.00 CA GLU C3050 13.344 7.735 16.187 1.00 27.21 CA GLU C3050 13.344 7.735 16.187 1.00 27.77 CA GLU C3051 13.342 12.486 12.946 1.00 28.83 CA GLU C3050 13.344 7.735 16.187 1.00 28.86 CA GLU C3050 13.344 7.735 16.187 1.00 28.66 CA GLU C3050 13.344 7.735 16.187 1.00 28.66 CA GLU C3050 13.344 7.735 16.187 1.00 28 | | | | | | | | | | 1.00 35 | .41 | C |
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| ATOM 2207 CE1 TYR C3051 13.712 8.371 13.904 1.00 26.96 C ATOM 2208 CD2 TYR C3051 11.127 9.373 13.809 1.00 27.47 C ATOM 2209 CE2 TYR C3051 11.593 8.788 14.967 1.00 27.13 C ATOM 2210 CZ TYR C3051 12.885 8.290 15.014 1.00 27.21 C ATOM 2211 OH TYR C3051 13.344 7.735 16.187 1.00 27.00 O ATOM 2212 C TYR C3051 13.344 7.735 16.187 1.00 27.00 O ATOM 2213 O TYR C3051 13.342 12.486 12.946 1.00 28.83 O ATOM 2214 N LEU C3052 13.886 12.063 10.812 1.00 28.73 N ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.73 N ATOM 2216 CB LEU C3052 16.105 12.059 9.761 1.00 27.77 C ATOM 2217 CG LEU C3052 17.603 12.372 9.816 1.00 27.77 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2222 N ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.521 15.881 10.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 16.168 10.738 1.00 26.76 C ATOM 2222 C ALA C3053 14.704 15.831 12.510 1.00 26.76 C ATOM 2223 CA ALA C3053 14.704 15.831 12.510 1.00 26.76 C ATOM 2224 CB ALA C3053 14.704 15.831 12.510 1.00 26.76 C ATOM 2225 C ALA C3053 14.704 15.831 12.510 1.00 26.76 C ATOM 2226 C ALA C3055 13.898 16.852 9.691 1.00 26.76 C ATOM 2227 N GLY C3054 13.512 15.753 14.934 1.00 26.77 N ATOM 2228 CA ALA C3055 13.898 16.852 9.691 1.00 26.76 C ATOM 2227 N ALA C3055 13.898 16.852 9.691 1.00 26.77 N ATOM 2228 CA ALA C3055 13.898 16.852 9.691 1.00 26.77 N ATOM 2228 CA ALA C3055 13.898 16.852 9.691 1.00 26.77 N ATOM 2230 CA ALA C3055 13.898 16.852 9.691 1.00 26.77 N ATOM 2231 N ARG C3055 13.898 16.852 9.691 1.00 26.69 N ATOM 2232 CA ARG C3055 | | | | | | | | | | | | |
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| ATOM 2211 OH IN C3051 13.019 12.117 11.818 1.00 29.01 C ATOM 2213 O TYR C3051 13.049 12.486 12.946 1.00 28.83 O ATOM 2214 N LEU C3052 13.886 12.063 10.812 1.00 28.07 C ATOM 2216 CB LEU C3052 15.287 12.417 11.009 1.00 28.07 C ATOM 2216 CB LEU C3052 16.105 12.059 9.761 1.00 28.07 C ATOM 2217 CG LEU C3052 17.603 12.372 9.816 1.00 28.06 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 10.0 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2225 C ALA C3053 14.231 16.489 12.134 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.130 15.831 12.510 1.00 26.67 C ATOM 2229 C GLY C3054 13.130 15.831 12.510 1.00 26.67 C ATOM 2230 CA ARG C3055 14.231 14.643 14.836 1.00 26.67 C ATOM 2231 N ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2231 N ARG C3055 15.198 14.290 15.870 1.00 26.69 N ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.69 N ATOM 2234 CG ARG C3055 15.198 14.290 15.870 1.00 26.69 C ATOM 2235 CD ARG C3055 15.198 14.290 15.870 1.00 26.96 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.76 C ATOM 2238 NH2 ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH2 ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH2 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2238 NH2 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.660 15.667 16.928 1.00 26.96 C | MOTA | | cz | | | | | | | | | |
| ATOM 2213 O TYR C3051 13.342 12.486 12.946 1.00 28.83 O ATOM 2214 N LEU C3052 13.886 12.063 10.812 1.00 28.73 N ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.07 C ATOM 2216 CB LEU C3052 16.105 12.059 9.761 1.00 27.77 C ATOM 2217 CG LEU C3052 17.603 12.372 9.816 1.00 28.06 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 10.00 27.06 N ATOM 2223 CA ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2224 CB ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2225 C ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2225 C ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2225 C ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2225 C ALA C3053 14.704 14.727 10.544 10.00 26.76 C ATOM 2225 C ALA C3053 14.898 16.852 9.691 1.00 26.76 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.76 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.77 N ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2230 O GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.66 N ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.68 C ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.68 C ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.66 C ATOM 2233 CB ARG C3055 15.198 11.843 16.498 1.00 26.96 C ATOM 2233 CB ARG C3055 15.795 11.100 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.665 1.00 27.69 N ATOM 2233 CB ARG C3055 11.4968 11.843 16.698 1.00 27.51 N ATOM 2233 NA 2RG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.665 1.00 27.51 N ATOM 2238 NH2 ARG C3055 10.662 11.831 16.667 10.00 27.71 N ATOM 2238 NH2 ARG C3055 10.662 11.831 16.667 10.00 27.71 N | ATOM | 2211 | OH | | | | | | | | | |
| ATOM 2214 N LEU C3052 13.886 12.063 10.812 1.00 28.73 N ATOM 2215 CA LEU C3052 15.287 12.417 11.009 1.00 28.07 C ATOM 2216 CB LEU C3052 16.105 12.059 9.761 1.00 27.77 C ATOM 2217 CG LEU C3052 17.603 12.372 9.816 1.00 28.06 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2224 CB ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2225 C ALA C3053 14.28 16.885 9.691 1.00 26.56 C ATOM 2226 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2229 C ARG C3055 14.231 14.643 14.836 1.00 26.667 C ATOM 2230 N ARG C3055 15.5198 14.290 15.880 1.00 26.667 C ATOM 2231 N ARG C3055 15.5198 14.290 15.880 1.00 26.665 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.65 C ATOM 2237 CZ ARG C3055 12.759 11.110 17.292 1.00 27.669 N ATOM 2238 NA ARG C3055 14.968 11.843 16.498 1.00 27.76 C ATOM 2237 CZ ARG C3055 12.759 11.110 17.292 1.00 27.669 N ATOM 2238 NA ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2238 NA ARG C3055 12.759 11.110 17.292 1.00 27.669 N ATOM 2238 NA ARG C3055 12.759 11.110 17.292 1.00 27.669 N ATOM 2239 NA ARG C3055 10.906 10.324 18.398 1.00 26.54 O ATOM 2239 NA ARG C3055 10.906 10.324 18.398 1.00 26.54 O ATOM 2239 NA ARG C3055 16.834 15.667 16.928 1.00 26.54 O ATOM 2230 NA ARG C3055 16.836 15.667 16.928 1.00 26.56 C ATOM 2231 NA ARG C3055 10.906 10.324 18.398 1.00 26.56 C ATOM 2239 NA ARG C3055 16.836 15.667 16.928 1.00 26.54 O ATOM 2241 O ARG C3055 16.836 15.667 16.928 1.00 26.54 O ATOM 2241 O ARG C3055 16.836 15.667 16.928 1.00 26.54 O AT | MOTA | 2212 | С | | | | | | | | | |
| ATOM 2214 N LEU C3052 15.287 12.417 11.009 1.00 28.07 C ATOM 2216 CB LEU C3052 16.105 12.059 9.761 1.00 27.77 C ATOM 2217 CG LEU C3052 17.603 12.372 9.816 1.00 28.06 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.267 11.639 10.972 1.00 28.46 C ATOM 2210 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2222 N ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 13.898 16.852 9.691 1.00 26.56 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2226 O ALA C3053 14.23 16.489 12.134 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.130 15.831 12.510 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.57 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2230 O GLY C3055 14.231 14.643 14.836 1.00 26.67 C ATOM 2231 N ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.66 C ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.69 C ATOM 2234 CG ARG C3055 13.468 11.922 16.298 1.00 27.49 C ATOM 2237 CZ ARG C3055 13.468 11.922 16.298 1.00 27.49 C ATOM 2238 NH1 ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.59 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.51 N ATOM 2237 CZ ARG C3055 10.906 10.324 18.398 1.00 27.51 N ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.966 C ATOM 2239 NH2 ARG C3055 16.360 15.260 15.869 1.00 26.966 C ATOM 2241 O ARG C3055 16.360 15.260 15.869 1.00 26.966 C | ATOM | 2213 | 0 | | | | | | | | | |
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| ATOM 2216 CB LBU C3052 17.603 12.372 9.816 1.00 28.06 C ATOM 2218 CD1 LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 0 LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2225 C ALA C3053 14.802 17.298 12.854 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.43 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.44 O ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.91 C ATOM 2234 CG ARG C3055 14.968 11.643 16.498 1.00 26.69 C ATOM 2235 CD ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2236 NE ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2237 NERG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2238 NH1 ARG C3055 14.968 11.843 16.498 1.00 27.49 C ATOM 2238 NH1 ARG C3055 14.968 11.843 16.498 1.00 27.49 C ATOM 2238 NH1 ARG C3055 14.968 11.843 16.498 1.00 27.49 C ATOM 2238 NH1 ARG C3055 14.968 11.843 16.498 1.00 27.69 N ATOM 2238 NH1 ARG C3055 10.966 10.324 18.398 1.00 27.51 N ATOM 2238 NH1 ARG C3055 10.966 10.324 18.398 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.966 10.324 18.398 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.966 10.324 18.398 1.00 26.96 C ATOM 2241 O ARG C3055 10.966 10.324 18.398 1.00 26.96 C | MOTA | 2215 | CA | | | | | | | | | |
| ATOM 2217 CB LEU C3052 18.267 11.639 10.972 1.00 28.26 C ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2222 CA ALA C3053 14.704 14.727 10.544 1.00 27.06 C ATOM 2224 CB ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2225 C ALA C3053 14.802 17.298 12.854 1.00 26.56 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2230 O GLY C3054 13.512 15.753 14.934 1.00 26.66 C ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2231 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2231 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.99 N ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.96 C ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.96 C ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 27.51 N ATOM 2241 O ARG C3055 16.360 15.667 16.928 1.00 27.71 | MOTA | 2216 | CB | | | | | | | | | |
| ATOM 2219 CD2 LEU C3052 18.241 11.957 8.516 1.00 28.46 C ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 C ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.56 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2236 NE ARG C3055 11.458 11.922 16.298 1.00 27.49 C ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.751 N ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 27.751 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 27.751 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 27.751 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 27.751 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.96 C ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.77 N ATOM 2241 O ARG C3055 16.360 15.660 15.869 1.00 26.96 C | MOTA | 2217 | | | | | | | | | | |
| ATOM 2220 C LEU C3052 15.419 13.909 11.311 1.00 27.59 ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 14.223 16.489 12.134 1.00 26.56 C ATOM 2225 C ALA C3053 14.802 17.298 12.854 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 O ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.44 O ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.66 N ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 12.759 11.110 17.292 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2238 NH1 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.56 C ATOM 2239 NH2 ARG C3055 16.360 15.260 15.869 1.00 27.51 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.76 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N | MOTA | 2218 | | | | | | | | | | |
| ATOM 2221 O LEU C3052 16.156 14.309 12.217 1.00 26.99 O ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2222 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2225 C ALA C3053 14.823 16.489 12.134 1.00 26.71 C ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2230 O GLY C3054 13.512 15.753 14.934 1.00 26.67 C ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.91 C ATOM 2233 CB ARG C3055 15.198 14.290 15.870 1.00 26.91 C ATOM 2234 CG ARG C3055 15.198 14.290 15.870 1.00 26.91 C ATOM 2236 NE ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2237 CZ ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2238 NH1 ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2238 NH1 ARG C3055 10.662 11.381 16.685 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.381 16.685 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2240 C ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2240 C ARG C3055 10.662 11.381 16.685 1.00 27.51 N ATOM 2240 C ARG C3055 10.662 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.360 15.260 15.869 1.00 26.54 O | MOTA | 2219 | CD2 | | | | | | | | | |
| ATOM 2222 N ALA C3053 14.704 14.727 10.544 1.00 27.06 N ATOM 2223 CA ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 13.898 16.852 9.691 1.00 26.56 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 O ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.76 C ATOM 2238 NH2 ARG C3055 10.906 10.324 18.398 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2239 NH2 ARG C3055 16.836 15.660 15.869 1.00 27.51 N ATOM 2240 C ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2240 C ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.836 15.661 16.928 1.00 26.54 | MOTA | 2220 | С | | | | | | | | | |
| ATOM 2222 N ALA C3053 14.743 16.168 10.738 1.00 26.76 C ATOM 2224 CB ALA C3053 13.898 16.852 9.691 1.00 26.56 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 O ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.67 C ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2235 CD ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.76 C ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 26.96 C ATOM 2240 C ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2240 C ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2221 | 0 | | | | | | | | | |
| ATOM 2224 CB ALA C3053 13.898 16.852 9.691 1.00 26.56 C ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 O ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 O ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 N ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2222 | N | | | | | | | | | |
| ATOM 2225 C ALA C3053 14.223 16.489 12.134 1.00 26.71 C ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 O ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 N ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.68 N ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 O | MOTA | 2223 | CA | | | | | | | | | |
| ATOM 2226 O ALA C3053 14.802 17.298 12.854 1.00 26.43 ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 ATOM 2231 N ARG C3055 15.198 14.290 15.870 1.00 26.82 ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 | ATOM | 2224 | CB | | | | | | | | | |
| ATOM 2227 N GLY C3054 13.130 15.831 12.510 1.00 26.77 ATOM 2228 CA GLY C3054 12.541 16.043 13.815 1.00 26.67 ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 27.71 | MOTA | | С | | | | | | | | | |
| ATOM 2228 CA GLY C3054 13.513 13.815 1.00 26.67 C ATOM 2229 C GLY C3054 13.512 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 O ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2226 | 0 | | | | | | | | | |
| ATOM 2228 CA GLY C3054 12.51 15.753 14.934 1.00 26.53 C ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 O ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 O ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2227 | N | | | | | | | | | |
| ATOM 2230 O GLY C3054 13.611 16.521 15.882 1.00 26.44 ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | | | | | | | | | | | |
| ATOM 2231 N ARG C3055 14.231 14.643 14.836 1.00 26.68 N ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2229 | С | | | | | | | | | |
| ATOM 2232 CA ARG C3055 15.198 14.290 15.870 1.00 26.82 C ATOM 2233 CB ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.54 O ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2230 | 0 | | | | | | | | | |
| ATOM 2232 CA ARG C3055 15.705 12.868 15.666 1.00 26.65 C ATOM 2234 CG ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2231 | N | | | | | | | 1.00 | 26.68 | |
| ATOM 2233 CB ARG C3055 14.968 11.843 16.498 1.00 26.91 C ATOM 2235 CD ARG C3055 13.458 11.922 16.298 1.00 27.49 C ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 N | ATOM | 2232 | CA | | | | | | | | | |
| ATOM 2234 CG ARG C3055 14.966 11.042 16.298 1.00 27.49 ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.69 N ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 | MOTA | 2233 | CB | | | | | | | | | |
| ATOM 2235 CD ARG C3055 13.436 11.322 1.00 27.69 N ATOM 2236 NE ARG C3055 12.759 11.110 17.292 1.00 27.76 C ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 N | MOTA | 2234 | CG | | | | | | | | | |
| ATOM 2237 CZ ARG C3055 11.442 11.086 17.454 1.00 27.76 C ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 N | ATOM | 2235 | CD | | | | | | | | | |
| ATOM 2237 CZ ARG C3055 11.442 11.000 17.51 N ATOM 2238 NH1 ARG C3055 10.662 11.831 16.685 1.00 27.51 N ATOM 2239 NH2 ARG C3055 10.906 10.324 18.398 1.00 28.13 N ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 O | ATOM | 2236 | NE | | | | | | | | | |
| ATOM 2238 NH1 ARG C3055 10.002 11.002 10.002 | ATOM | 2237 | | | | | | | | | | |
| ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 C ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 O | ATOM | 2238 | | | | | | | | | | |
| ATOM 2240 C ARG C3055 16.360 15.260 15.869 1.00 26.96 ATOM 2241 O ARG C3055 16.834 15.667 16.928 1.00 26.54 O | ATOM | 2239 | NH | | | | | | | | | |
| ATOM 2241 0 TAKE 050 15 C71 14 C7C 1 00 27 71 N | | 2240 | С | | | | | | | | | |
| +c 0+c 1F C31 14 676 1 00 77 71 | | 2241 | Ó | | | | | | | | | |
| | MOTA | 2242 | N | TR | P C3056 | | 16.816 | 15.631 | 14.6/6 | 1.00 | 21.11 | 1.4 |

| ATOM | 2243 | CA | TRP (| C3056 | | 17.917 | 16.575 | 14.556 | 1.00 | 28.70 | С |
|--------------|------|----|-------|---------|---|--------|--------|---------|------|---------|---|
| ATOM | 2244 | СВ | | C3056 | | 18.247 | 16.837 | 13.082 | 1.00 | 30.14 | С |
| ATOM | 2245 | CG | | C3056 | | 19.074 | 18.069 | 12.881 | 1.00 | 32.25 | С |
| ATOM | 2246 | | | C3056 | | 20.495 | 18.129 | 12.703 | 1.00 | 33.03 | С |
| ATOM | 2247 | | | C3056 | | 20.854 | 19.497 | 12.662 | | 33.33 | С |
| | | | | C3056 | | 21.500 | 17.163 | 12.579 | | 33.56 | С |
| ATOM | 2248 | | | | | 18.639 | 19.370 | 12.930 | | 32.92 | С |
| ATOM | 2249 | | | C3056 | | | 20.230 | 12.803 | | 33.50 | N |
| MOTA | 2250 | | | C3056 | | 19.704 | 19.920 | 12.505 | | 33.41 | C |
| ATOM | 2251 | | | C3056 | | 22.175 | | 12.422 | | 33.92 | Ċ |
| ATOM | 2252 | | | C3056 | | 22.818 | 17.587 | 12.422 | | 33.82 | Č |
| ATOM | 2253 | | | C3056 | | 23.141 | 18.954 | | | 28.10 | Ċ |
| ATOM | 2254 | C | | C3056 | | 17.498 | 17.875 | 15.230 | | | 0 |
| MOTA | 2255 | 0 | | C3056 | | 18.144 | 18.357 | 16.163 | | 27.48 | |
| MOTA | 2256 | N | SER | C3057 | | 16.397 | 18.429 | 14.749 | | 27.65 | N |
| ATOM | 2257 | CA | | C3057 | | 15.868 | 19.667 | 15.288 | | 27.54 | C |
| ATOM | 2258 | CB | SER | C3057 | | 14.513 | 19.959 | 14.654 | | 27.86 | |
| ATOM | 2259 | OG | SER | C3057 | | 14.233 | 21.344 | 14.718 | | 29.93 | 0 |
| ATOM | 2260 | С | SER | C3057 | | 15.731 | 19.622 | 16.812 | | 26.85 | C |
| ATOM | 2261 | 0 | SER | C3057 | | 16.059 | 20.588 | 17.503 | | 27.24 | 0 |
| ATOM | 2262 | N | ALA | C3058 | | 15.257 | 18.501 | 17.340 | | 25.77 | N |
| ATOM | 2263 | CA | ALA | C3058 | | 15.080 | 18.369 | 18.780 | 1.00 | 25.50 | С |
| ATOM | 2264 | CB | ALA | C3058 | | 14.334 | 17.077 | 19.094 | | 25.02 | С |
| ATOM | 2265 | С | ALA | C3058 | | 16.411 | 18.409 | 19.546 | | 25.26 | С |
| ATOM | 2266 | Ō | | C3058 | | 16.513 | 19.024 | 20.607 | 1.00 | 24.25 | 0 |
| ATOM | 2267 | N | | C3059 | | 17.430 | 17.752 | 19.000 | 1.00 | 25.32 | N |
| ATOM | 2268 | CA | | C3059 | | 18.736 | 17.704 | 19.646 | 1.00 | 25.14 | C |
| ATOM | 2269 | CB | | C3059 | | 19.568 | 16.577 | 19.035 | 1.00 | 24.87 | С |
| ATOM | 2270 | CG | | C3059 | • | 18.928 | 15.218 | 19.254 | 1.00 | 24.63 | С |
| ATOM | 2271 | CD | | C3059 | | 19.667 | 14.091 | 18.570 | 1.00 | 24.80 | C |
| ATOM | 2272 | CE | | C3059 | | 18.998 | 12.746 | 18.869 | 1.00 | 24.92 | C |
| ATOM | 2273 | NZ | | C3059 | | 19.674 | 11.614 | 18.185 | 1.00 | 24.83 | N |
| ATOM | 2274 | C | | C3059 | | 19.466 | 19.033 | 19.547 | 1.00 | 25.56 | С |
| ATOM | 2275 | Ö | | C3059 | | 20.262 | 19.383 | 20.415 | 1.00 | 25.33 | 0 |
| ATOM | 2276 | N | | C3060 | | 19.183 | 19.784 | 18.493 | 1.00 | 26.00 | N |
| ATOM | 2277 | CA | | C3060 | | 19.818 | 21.076 | 18.326 | 1.00 | 26.76 | С |
| ATOM | 2278 | СВ | | C3060 | | 19.568 | 21.618 | `16.919 | 1.00 | 28.10 | С |
| ATOM | 2279 | CG | | C3060 | | 20.545 | 22.717 | 16.530 | 1.00 | 31.38 | С |
| ATOM | 2280 | CD | | C3060 | | 22.005 | 22.278 | 16.691 | 1.00 | 33.19 | С |
| ATOM | 2281 | | | C3060 | | 22.444 | 21.369 | 15.947 | 1.00 | 33.60 | 0 |
| MOTA | 2282 | | | C3060 | | 22.709 | 22.839 | 17.569 | 1.00 | 34.17 | 0 |
| ATOM | 2283 | C | | C3060 | | 19.243 | 22.023 | 19.377 | 1.00 | 26.31 | С |
| ATOM | 2284 | ō | | C3060 | | 19.985 | 22.698 | 20.089 | 1.00 | 25.94 | 0 |
| ATOM | 2285 | N | | C3061 | | 17.914 | 22.048 | 19.477 | 1.00 | 25.95 | N |
| ATOM | 2286 | CA | | C3061 | | 17,221 | 22.899 | 20.442 | 1.00 | 25.01 | С |
| ATOM | 2287 | | | C3061 | | | | 20.342 | 1.00 | 24.05 | С |
| ATOM | 2288 | | | C3061 | | 17.696 | 22.562 | 21.846 | 1.00 | 24.62 | С |
| ATOM | 2289 | | | C3061 | | 17.925 | | | | 24.28 | 0 |
| MOTA | 2290 | | | C3062 | | 17.837 | | | | 24.17 | N |
| ATOM | 2291 | | | C3062 | | 18.301 | | | 1.00 | 24.63 | С |
| MOTA | 2292 | | | C3062 | | 18.224 | | 23.605 | 1.00 | 24.68 | С |
| | 2292 | | | C3062 | | 18.875 | | | | 24.04 | С |
| MOTA | 2293 | | | C3062 | | 20.238 | | | | 24.34 | С |
| ATOM | 2294 | | | C3062 | | 18.152 | | | | 0 23.91 | С |
| ATOM ATOM | 2295 | | | C3062 | | 20.872 | | | | 0 24.30 | С |
| ATOM | 2297 | | | C3062 | | 18.774 | | | | 0 24.14 | С |
| ATOM | 2298 | | | C3062 | | 20.139 | | | | 0 24.07 | С |
| ATOM | 2299 | | | C3062 | | 19.732 | | | | 0 24.85 | С |
| AIOM | 2273 | | - +1 | . 00002 | | | | | | | |

| ATOM | 2300 | 0 | PHE | C3062 | 20.054 | 21.744 | | 1.00 | | 0 |
|--------------|--------------|---|-----|----------------|------------------|----------|------------------|-------|--------------------|--------|
| ATOM | 2301 | N | SER | C3063 | 20.589 | 21.219 | 22.689 | 1.00 | | N |
| ATOM | 2302 | CA | SER | C3063 | 21.976 | 21.650 | 22.833 | 1.00 | | С |
| ATOM | 2303 | CB | SER | C3063 | 22.777 | 21.312 | 21.576 | 1.00 | | C |
| ATOM | 2304 | OG | SER | C3063 | 22.872 | 19.910 | 21.403 | 1.00 | | 0 |
| ATOM | 2305 | C | SER | C3063 | 22.059 | 23.149 | 23.082 | 1.00 | | С |
| ATOM | 2306 | 0 | SER | C3063 | 22.891 | 23.614 | 23.859 | 1.00 | | 0 |
| ATOM | 2307 | N | LYS | C3064 | 21.194 | 23.902 | 22.416 | 1.00 | 26.78 | N |
| MOTA | 2308 | CA | LYS | C3064 | 21.188 | 25.342 | 22.565 | | 27.25 | С |
| MOTA | 2309 | CB | LYS | C3064 | 20.379 | 25.973 | 21.431 | | 26.90 | C |
| MOTA | 2310 | CG | LYS | C3064 | 20.971 | 25.696 | 20.059 | | 26.47 | C |
| ATOM | 2311 | CD | | C3064 | 20.066 | 26.159 | 18.938 | | 26.20 | C |
| ATOM | 2312 | CE | LYS | C3064 | 19.799 | 27.664 | 18.988 | | 26.50 | C |
| MOTA | 2313 | NZ | | C3064 | 18.996 | 28.088 | 17.806 | | 26.49 | N C |
| MOTA | 2314 | С | | C3064 | 20.616 | 25.718 | 23.923 | | 28.08 | 0 |
| MOTA | 2315 | 0 | | C3064 | 20.987 | 26.738 | 24.500 | | 27.79 | Ŋ |
| ATOM | 2316 | N | | C3065 | 19.717 | 24.882 | 24.433 | | 29.11 | C |
| MOTA | 2317 | CA | | C3065 | 19.111 | 25.124 | 25.735 | | 30.40 | c |
| MOTA | 2318 | CB | | C3065 | 17.957 | 24.163 | 25.968 | | 29.37 31.79 | C |
| MOTA | 2319 | С | | C3065 | 20.179 | | 26.804 | | 31.75 | Ö |
| MOTA | 2320 | 0 | | C3065 | 20.228 | 25.668 | 27.786 | | 33.85 | N |
| MOTA | 2321 | N | | C3066 | 21.035 | 23.939 | 26.595 27.524 | | 36.16 | C |
| MOTA | 2322 | CA | | C3066 | 22.114 | 23.628 | | | 36.40 | C |
| MOTA | 2323 | CB | | C3066 | 22.666 | | 27.242 27.752 | | 37.31 | c |
| MOTA | 2324 | CG | | C3066 | 21.804 | | 29.551 | | 38.61 | s |
| MOTA | 2325 | SD | | C3066 | 21.824 | | 29.331 | | 38.12 | c |
| MOTA | 2326 | CE | | C3066 | 23.502 | | 27.413 | | 37.57 | c |
| MOTA | 2327 | С | | C3066 | 23.247 | | 28.379 | | 37.83 | Ō |
| MOTA | 2328 | 0 | | C3066 | 23.958 | | 26.226 | | 39.17 | N |
| MOTA | 2329 | N | | C3067 | 23.411 24.470 | | 26.024 | | 41.14 | C |
| MOTA | 2330 | CA | | C3067 | 25.772 | | 25.697 | | 42.59 | С |
| ATOM | 2331 | C | | C3067 C3067 | 26.831 | | 26.226 | | 42.74 | 0 |
| ATOM | 2332 | 0 | | C3067 | 25.687 | | 24.825 | | 43.64 | N |
| ATOM | 2333 | N | | R C3068 | 26.853 | | 24.418 | | 44.94 | С |
| ATOM | 2334 | CA CB | | R C3068 | 26.723 | _ | 24.877 | | 45.62 | C |
| ATOM ATOM | 2335 2336 | | | R C3068 | 27.927 | | 24.559 | | 46.68 | 0 |
| MOTA | 2337 | | | R C3068 | 25.539 | | | | 45.83 | С |
| ATOM | 2338 | C. | | R C3068 | 26.994 | | | 1.00 | 45.32 | С |
| ATOM | 2339 | o | | R C3068 | 26.027 | | 22.242 | | 45.93 | 0 |
| MOTA | 2340 | | | R C3068 | 28.057 | 23.348 | 22.377 | 1.00 | 45.68 | 0 |
| TER | 2341 | • | | R C3068 | | | | | | _ |
| ATOM | 2342 | С | GL' | Y C3074 | 25.582 | 13.730 | | | 50.05 | C |
| ATOM | 2343 | | | Y C3074 | 24.831 | | | | 50.04 | 0 |
| MOTA | | | GL | Y C3074 | 27.008 | 15.502 | 22.091 | | 50.49 | N |
| ATOM | 2345 | | | Y C3074 | 26.990 | | | | 50.33 | C |
| MOTA | 2346 | | PH | E C3075 | 25.218 | 3 13.780 | | | 49.73 | N |
| MOTA | 2347 | CA | PH | E C3075 | 23.894 | | | | 49.39 | C |
| MOTA | 2348 | CB | PH | E C3075 | 23.740 | | | | 49.61 | C |
| ATOM | 2349 | | | E C3075 | 23.19 | | | | 50.02 | C C |
| ATOM | 2350 | | | E C3075 | 23.55 | | | | 50.35 | C |
| MOTA | 2351 | | | E C3075 | 22.31 | | | | 50.13 | C |
| ATOM | 2352 | | | E C3075 | 23.04 | | | | 0 50.43 | C |
| MOTA | 2353 | | | E C3075 | 21.79 | | | | 0 50.56 | C |
| MOTA | 2354 | | | E C3075 | | | | | 0 50.60 0 48.79 | C |
| ATOM | 2355 | | | E C3075 | | | | | 0 48.79 | 0 |
| MOTA | 235€ | 5 0 | PH | E C3075 | 22.53 | 0 11.523 | 3 20.07 | 5 1.0 | 0 40.55 | J |
| | | | | | | | | | | |

| ATOM | 2357 | N GI | LN C3076 | 24.694 | 11.082 | 19.642 | 1.00 48.39 | N |
|------|------|-------|-----------|--------|---------|--------|--------------|--------|
| ATOM | 2358 | CA GI | LN C3076 | 24.602 | 9.671 | 19.998 | 1.00 47.89 | C |
| ATOM | 2359 | CB GI | LN C3076 | 25.905 | 8.944 | 19.643 | 1.00 48.47 | С |
| ATOM | 2360 | CG GI | LN C3076 | 26.287 | 9.049 | 18.175 | 1.00 49.29 | C |
| ATOM | 2361 | | LN C3076 | 25.242 | 8.441 | 17.260 | 1.00 49.81 | С |
| ATOM | 2362 | | LN C3076 | 25.206 | 8.731 | 16.065 | 1.00 50.75 | 0 |
| ATOM | 2363 | | LN C3076 | 24.391 | 7.584 | 17.815 | 1.00 49.76 | N |
| ATOM | 2364 | | LN C3076 | 24.351 | 9.560 | 21.492 | 1.00 47.10 | С |
| ATOM | 2365 | | LN C3076 | 24.003 | 8.493 | 22.000 | 1.00 47.45 | 0 |
| ATOM | 2366 | | SP C3077 | 24.533 | 10.676 | 22.190 | 1.00 45.97 | N |
| ATOM | 2367 | | SP C3077 | 24.331 | 10.727 | 23.631 | 1.00 44.90 | С |
| | 2368 | | SP C3077 | 25.397 | 11.612 | 24.271 | 1.00 46.44 | С |
| ATOM | 2369 | | SP C3077 | 26.800 | 11.083 | 24.036 | 1.00 47.82 | С |
| ATOM | | | SP C3077 | 27.081 | 9.951 | 24.499 | 1.00 48.20 | 0 |
| ATOM | 2370 | | SP C3077 | 27.610 | 11.794 | 23.388 | 1.00 48.48 | 0 |
| ATOM | 2371 | | SP C3077 | 22.950 | 11.252 | 23.975 | 1.00 43.23 | С |
| MOTA | 2372 | | SP C3077 | 22.557 | 11.280 | 25.140 | 1.00 43.47 | 0 |
| ATOM | 2373 | | EU C3078 | 22.219 | 11.675 | 22.950 | 1.00 41.15 | N |
| ATOM | 2374 | | | 20.869 | 12.193 | 23.129 | 1.00 38.63 | С |
| ATOM | 2375 | | EU C3078 | 20.754 | 13.610 | 22.558 | 1.00 38.12 | С |
| MOTA | 2376 | | EU C3078 | | 14.645 | 23.005 | 1.00 37.91 | · C |
| MOTA | 2377 | | EU C3078 | 21.787 | 15.974 | 22.313 | 1.00 37.65 | С |
| ATOM | 2378 | | EU C3078 | 21.511 | | 24.508 | 1.00 37.75 | Ċ |
| ATOM | 2379 | | EU C3078 | 21.735 | 14.801 | 22.376 | 1.00 36.97 | Ċ |
| ATOM | 2380 | | EU C3078 | 19.921 | 11.272 | 21.269 | 1.00 36.76 | ő |
| ATOM | 2381 | _ | EU C3078 | 20.225 | 10.833 | | 1.00 34.99 | N |
| MOTA | 2382 | | LU C3079 | 18.778 | 10.974 | 22.979 | 1.00 34.33 | C |
| MOTA | 2383 | | LU C3079 | 17.793 | 10.112 | 22.338 | 1.00 33.32 | Č |
| MOTA | 2384 | | SLU C3079 | 17.937 | 8.676 | 22.842 | | c |
| MOTA | 2385 | | SLU C3079 | 16.818 | 7.753 | 22.412 | 1.00 34.12 | c |
| ATOM | 2386 | | GLU C3079 | 17.129 | 6.298 | 22.691 | 1.00 34.85 | . 0 |
| MOTA | 2387 | | GLU C3079 | 17.897 | 5.701 | 21.908 | 1.00 34.18 | 0 |
| MOTA | 2388 | - | GLU C3079 | 16.616 | 5.754 | 23.699 | 1.00 35.70 | c |
| ATOM | 2389 | | SLU C3079 | 16.365 | 10.598 | 22.566 | 1.00 31.51 | Ö |
| ATOM | 2390 | - | GLU C3079 | 15.955 | 10.880 | 23.695 | 1.00 31.00 | Ŋ |
| ATOM | 2391 | | VAL C3080 | 15.618 | 10.707 | 21.474 | 1.00 29.65 | C |
| ATOM | 2392 | CA V | VAL C3080 | 14.237 | 11.135 | 21.542 | 1.00 28.33 | C |
| ATOM | 2393 | | VAL C3080 | 13.987 | 12.401 | 20.698 | 1.00 28.04 | C |
| ATOM | 2394 | CG1 V | VAL C3080 | 12.497 | 12.701 | 20.643 | 1.00 27.55 | c |
| ATOM | 2395 | CG2 1 | VAL C3080 | 14.739 | 13.576 | 21.289 | 1.00 27.56 | c |
| MOTA | 2396 | C ' | VAL C3080 | 13.373 | | 21.007 | 1.00 28.05 | 0 |
| MOTA | 2397 | 0 ' | VAL C3080 | 13.518 | 9.600 | | 1.00 27.43 | |
| MOTA | 2398 | | LEU C3081 | 12.482 | | | | И С |
| ATOM | 2399 | CA | LEU C3081 | 11.578 | | 21.455 | | C |
| ATOM | 2400 | | LEU C3081 | 11.724 | 7.235 | 22.391 | | C |
| ATOM | 2401 | | LEU C3081 | 13.107 | | | 1.00 27.65 | |
| ATOM | 2402 | CD1 | LEU C3081 | 13.069 | | | | C |
| MOTA | 2403 | CD2 | LEU C3081 | 13.534 | | | | C |
| MOTA | 2404 | С | LEU C3081 | 10.160 | | | | C |
| ATOM | 2405 | 0 | LEU C3081 | 9.965 | | | | 0 |
| MOTA | 2406 | N | ASN C3082 | 9.177 | | | | N |
| MOTA | 2407 | | ASN C3082 | 7.775 | | | | C |
| ATOM | 2408 | | ASN C3082 | 7.111 | 8.355 | | | C |
| ATOM | 2409 | | ASN C3082 | 7.584 | | | | C |
| MOTA | 2410 | | ASN C3082 | 7.295 | 10.569 | | 1.00 29.62 | 0 |
| ATOM | 2411 | | ASN C3082 | 8.321 | 8.932 | | | N |
| ATOM | 2412 | | ASN C3082 | 7.053 | 3 7.647 | | | C |
| ATOM | 2413 | | ASN C3082 | 7.199 | 6.421 | 22.40 | 7 1.00 28.06 | 0 |
| | | | | | | | | |

| ATOM | 2414 | N | ASN | C3083 | | 6.280 | 8.274 | 23.308 | 1.00 27.85 | | N |
|-------|------|-----|-------|-------|---|--------|--------|--------|------------|-----|----|
| ATOM | 2415 | CA | | C3083 | | 5.537 | 7.520 | 24.304 | 1.00 27.66 | | C |
| ATOM | 2416 | CB | | C3083 | | 5.183 | 8.398 | 25.515 | 1.00 27.64 | | Č |
| ATOM | 2417 | CG | | C3083 | | 4.203 | 9.527 | 25.189 | 1.00 27.67 | | Ċ |
| ATOM | 2418 | | | C3083 | | 3.949 | 10.384 | 26.033 | 1.00 28.51 | | Ö |
| | | | | C3083 | | 3.648 | 9.527 | 23.986 | 1.00 23.31 | | N |
| MOTA | 2419 | | | | | | | | 1.00 27.19 | | C |
| ATOM | 2420 | C | | C3083 | | 4.287 | 6.942 | 23.664 | | | |
| ATOM | 2421 | 0 | | C3083 | | 3.988 | 7.233 | 22.501 | 1.00 27.10 | | 0 |
| ATOM | 2422 | N | | C3084 | | 3.564 | 6.120 | 24.419 | 1.00 28.22 | | N |
| ATOM | 2423 | CA | | C3084 | | 2.354 | 5.483 | 23.910 | 1.00 28.64 | | C |
| ATOM | 2424 | CB | | C3084 | | 1.655 | 4.679 | 25.018 | 1.00 29.96 | | C |
| ATOM | 2425 | CG | | C3084 | | 1.146 | 5.509 | 26.187 | 1.00 31.56 | | C |
| MOTA | 2426 | CD | | C3084 | • | 2.225 | 5.820 | 27.210 | 1.00 33.17 | | C |
| ATOM | 2427 | | | C3084 | | 3.404 | 5.994 | 26.821 | 1.00 33.53 | | 0 |
| ATOM | 2428 | | | C3084 | | 1.888 | 5.903 | 28.411 | 1.00 34.64 | | 0 |
| ATOM | 2429 | С | | C3084 | | 1.367 | 6.471 | 23.291 | 1.00 28.20 | | С |
| ATOM | 2430 | 0 | | C3084 | | 0.559 | 6.092 | 22.446 | 1.00 28.01 | | 0 |
| ATOM | 2431 | N | ARG | C3085 | | 1.435 | 7.734 | 23.702 | 1.00 27.98 | | N |
| MOTA | 2432 | CA | | C3085 | | 0.526 | 8.745 | 23.165 | 1.00 27.80 | | С |
| ATOM | 2433 | CB | ARG | C3085 | | 0.270 | 9.847 | 24.201 | 1.00 28.19 | | С |
| ATOM | 2434 | CG | ARG | C3085 | | -0.474 | 9.355 | 25.427 | 1.00 29.28 | : | C |
| MOTA | 2435 | CD | ARG | C3085 | | -1.296 | 10.454 | 26.109 | 1.00 30.50 |) | C |
| MOTA | 2436 | NE | ARG | C3085 | | -2.245 | 9.862 | 27.052 | 1.00 31.26 | | N |
| MOTA | 2437 | CZ | ARG | C3085 | | -1.872 | 9.221 | 28.153 | 1.00 32.48 | ļ . | С |
| ATOM | 2438 | NH1 | ARG | C3085 | | -0.581 | 9.110 | 28.437 | 1.00 33.70 | 1 | N |
| ATOM | 2439 | NH2 | ARG | C3085 | | -2.770 | 8.663 | 28.954 | 1.00 33.05 | i | N |
| ATOM | 2440 | С | ARG | C3085 | | 1.021 | 9.369 | 21.863 | 1.00 27.34 | : | С |
| MOTA | 2441 | 0 | ARG | C3085 | | 0.310 | 10.158 | 21.244 | 1.00 27.35 | , | 0 |
| ATOM | 2442 | N | GLY | C3086 | | 2.237 | 9.016 | 21.454 | 1.00 26.82 | ? | N |
| ATOM | 2443 | CA | GLY | C3086 | | 2.788 | 9.545 | 20.218 | 1.00 25.87 | • | С |
| MOTA | 2444 | С | GLY | C3086 | | 3.607 | 10.808 | 20.384 | 1.00 25.74 | • | С |
| MOTA | 2445 | 0 | GLY | C3086 | | 4.109 | 11.370 | 19.401 | 1.00 25.82 | 2 | 0 |
| ATOM | 2446 | N | ALA | C3087 | | 3.753 | 11.254 | 21.626 | 1.00 24.99 | 5 | N |
| ATOM | 2447 | CA | ALA | C3087 | | 4.508 | 12.461 | 21.920 | 1.00 24.5 | 7 | С |
| ATOM | 2448 | СВ | | C3087 | | 3.933 | 13.147 | 23.155 | 1.00 24.64 | ļ | С |
| ATOM | 2449 | C | | C3087 | | 5.991 | 12.183 | 22.130 | 1.00 24.40 | ŝ | С |
| ATOM | 2450 | 0 | | C3087 | | 6.372 | 11.277 | 22.878 | 1.00 24.54 | ļ | 0 |
| ATOM | 2451 | N | | C3088 | | 6.851 | 12.964 | 21.461 | 1.00 24.09 | • | N |
| ATOM | 2452 | CD | | C3088 | | 6.501 | 14.011 | 20.482 | 1.00 23.73 | | С |
| ATOM | 2453 | CA | | C3088 | | 8.306 | 12.815 | 21.572 | 1.00 23.70 | 5 | С |
| ATOM | 2454 | CB | | C3088 | | 8.825 | 13.714 | 20.451 | 1.00 23.93 | | С |
| ATOM | 2455 | CG | | C3088 | | 7.781 | 14.816 | 20.403 | 1.00 23.82 | | С |
| ATOM | 2456 | C | | C3088 | | 8.799 | 13.249 | 22.952 | 1.00 23.43 | | С |
| ATOM | 2457 | 0 | | C3088 | | 8.162 | 14.066 | 23.610 | 1.00 23.0 | | 0 |
| MOTA | 2458 | N | | C3089 | | 9.925 | 12.692 | 23.391 | 1.00 23.7 | | N |
| ATOM | 2459 | CA | | C3089 | | 10.496 | 13.028 | 24.698 | 1.00 24.4 | | С |
| MOTA | 2460 | СВ | | C3089 | | 9.671 | 12.400 | 25.834 | 1.00 24.3 | | C |
| MOTA | 2461 | CG | | C3089 | | 9.843 | 10:904 | 25.973 | 1.00 24.6 | | С |
| ATOM | 2462 | | | C3089 | | 10.832 | 10.363 | 26.804 | 1.00 24.6 | • | С |
| ATOM | 2463 | | | C3089 | | 11.008 | 8.978 | 26.911 | 1.00 24.9 | | C |
| ATOM | 2464 | | | C3089 | | 9.033 | 10.027 | 25.256 | 1.00 24.8 | | C |
| ATOM | 2465 | | | C3089 | | 9.199 | 8.643 | 25.352 | 1.00 25.4 | | Ċ |
| ATOM | 2466 | CZ | | C3089 | | 10.187 | 8.125 | 26.178 | 1.00 25.3 | | č |
| ATOM | 2467 | OH | | C3089 | | 10.353 | 6.761 | 26.236 | 1.00 25.5 | | Õ |
| MOTA | 2468 | C | | C3089 | | 11.925 | 12.521 | 24.772 | 1.00 24.8 | | c |
| ATOM | 2469 | Ô | | C3089 | | 12.279 | 11.552 | 24.103 | 1.00 25.1 | | Õ |
| ATOM | 2470 | N | | C3090 | | 12.750 | 13.171 | 25.584 | 1.00 25.5 | | N |
| 71 OL | 24/0 | 1.7 | - 112 | ~JUJU | | 12.00 | 10.11 | 23.304 | 1,00 23.3 | - | ., |

| ATOM | 2471 | CA | PHE | C3090 | 14.135 | 12.742 | 25.714 | 1.00 26.19 | С |
|-----------|------|--------|-----|---------|--------|--------|--------|------------|--------|
| ATOM | 2472 | CB | | C3090 | 15.038 | 13.901 | 26.156 | 1.00 26.18 | С |
| ATOM | 2473 | CG | | C3090 | 15.387 | 14.852 | 25.051 | 1.00 26.76 | С |
| ATOM | 2474 | | | C3090 | 14.541 | 15.912 | 24.725 | 1.00 27.13 | Ċ |
| ATOM | 2475 | | | C3090 | 16.554 | 14.675 | 24.311 | 1.00 27.22 | Č |
| ATOM | 2476 | | | C3090 | 14.851 | 16.792 | 23.675 | 1.00 27.19 | Ċ |
| ATOM | 2477 | | | C3090 | 16.882 | 15.548 | 23.253 | 1.00 27.68 | č |
| ATOM | 2478 | CZ | | C3090 | 16.025 | 16.608 | 22.936 | 1.00 27.50 | c |
| ATOM | 2479 | C | | C3090 | 14.277 | 11.595 | 26.693 | 1.00 26.31 | Č |
| ATOM | 2480 | 0 | | C3090 | 14.076 | 11.767 | 27.895 | 1.00 27.02 | 0 |
| ATOM | | N | | C3091 | 14.616 | 10.423 | 26.169 | 1.00 26.64 | N |
| | 2481 | | | | | 9.237 | 26.994 | 1.00 20.04 | C |
| ATOM | 2482 | CA | | C3091 | 14.818 | | 26.185 | 1.00 27.10 | c |
| MOTA | 2483 | CB | | C3091 | 14.549 | 7.964 | | | |
| ATOM | 2484 | OG | | C3091 | 15.280 | 7.970 | 24.974 | 1.00 27.09 | 0 |
| ATOM | 2485 | C | | C3091 | 16.256 | 9.235 | 27.513 | 1.00 27.57 | C |
| ATOM | 2486 | 0 | | C3091 | 16.594 | 8.485 | 28.424 | 1.00 27.76 | 0 |
| ATOM | 2487 | N | | C3092 | 17.095 | 10.086 | 26.928 | 1.00 28.18 | N |
| ATOM | 2488 | CA | | C3092 | 18.490 | 10.199 | 27.340 | 1.00 29.06 | C |
| ATOM | 2489 | CB | | C3092 | 19.355 | 9.181 | 26.595 | 1.00 30.20 | С |
| ATOM | 2490 | CG | | C3092 | 20.843 | 9.363 | 26.840 | 1.00 31.72 | C |
| MOTA | 2491 | CD | GLN | C3092 | 21.280 | 8.873 | 28.211 | 1.00 32.79 | С |
| ATOM | 2492 | OE1 | GLN | C3092 | 21.336 | 7.667 | 28.461 | 1.00 33.66 | 0 |
| MOTA | 2493 | NE2 | GLN | C3092 | 21.590 | 9.805 | 29.105 | 1.00 33.12 | N |
| ATOM | 2494 | С | GLN | C3092 | 19.021 | 11.601 | 27.069 | 1.00 28.89 | C |
| MOTA | 2495 | 0 | GLN | C3092 · | 18.889 | 12.118 | 25.954 | 1.00 29.04 | 0 |
| MOTA | 2496 | N | ALA | C3093 | 19.630 | 12.207 | 28.088 | 1.00 28.63 | N |
| MOTA | 2497 | CA | ALA | C3093 | 20.179 | 13.556 | 27.963 | 1.00 28.35 | С |
| ATOM | 2498 | CB | ALA | C3093 | 19.040 | 14.565 | 27.805 | 1.00 28.23 | С |
| MOTA | 2499 | С | ALA | C3093 | 21.047 | 13.945 | 29.159 | 1.00 28.01 | С |
| ATOM | 2500 | 0 | | C3093 | 20.721 | 13.635 | 30.307 | 1.00 28.15 | 0 |
| ATOM | 2501 | N | PRO | C3094 | 22.167 | 14.640 | 28.905 | 1.00 27.81 | N |
| ATOM | 2502 | CD | | C3094 | 22.702 | 15.035 | 27.590 | 1.00 27.69 | С |
| ATOM | 2503 | CA | | C3094 | 23.066 | 15.067 | 29.984 | 1.00 27.41 | С |
| ATOM | 2504 | CB | | C3094 | 24.271 | 15.625 | 29.226 | 1.00 27.35 | С |
| ATOM | 2505 | CG | | C3094 | 23.658 | 16.148 | 27.960 | 1.00 27.34 | С |
| ATOM | 2506 | C | | C3094 | 22.409 | 16.108 | 30.883 | 1.00 27.24 | C |
| ATOM | 2507 | ō | | C3094 | 22.992 | 17.150 | 31.172 | 1.00 27.73 | 0 |
| ATOM | 2508 | N | | C3095 | 21.195 | 15.820 | 31.330 | 1.00 26.89 | N |
| ATOM | 2509 | CA | | C3095 | 20.457 | 16.740 | 32.182 | 1.00 26.88 | C |
| ATOM | 2510 | CB | | C3095 | 19.603 | 17.680 | 31.314 | 1.00 26.34 | C |
| ATOM | 2511 | CG | | C3095 | 18.986 | 18.820 | 32.081 | 1.00 25.69 | Ċ |
| ATOM | 2512 | | | C3095 | 19.789 | 19.707 | 32.796 | 1.00 24.82 | C |
| MOTA | 2513 | | | C3095 | 17.606 | 18.973 | 32.133 | 1.00 24.80 | Č |
| ATOM | 2514 | | | C3095 | 19.224 | 20.722 | 33.556 | 1.00 24.83 | Č |
| ATOM | 2515 | | | C3095 | 17.031 | 19.985 | 32.890 | 1.00 24.99 | Č |
| ATOM | 2516 | CZ | | C3095 | 17.841 | 20.862 | 33.605 | 1.00 24.98 | Č |
| ATOM | 2517 | C | | C3095 | 19.569 | 15.927 | 33.115 | 1.00 27.25 | č |
| ATOM | 2518 | Ö | | C3095 | 18.924 | 14:983 | 32.684 | 1.00 28.50 | o |
| ATOM | 2519 | И | | C3096 | 19.525 | 16.284 | 34.390 | 1.00 27.37 | N |
| ATOM ATOM | 2520 | CA | | C3096 | 18.710 | 15.530 | 35.332 | 1.00 27.95 | C |
| ATOM | 2521 | CB | | C3096 | 19.542 | 15.174 | 36.565 | 1.00 27.93 | Ċ |
| ATOM ATOM | 2521 | OG | | C3096 | 20.425 | 16.230 | 36.883 | 1.00 28.67 | 0 |
| | 2523 | C | | C3096 | 17.403 | 16.202 | 35.754 | 1.00 30.49 | . C |
| ATOM | | | | C3096 | 16.663 | | | 1.00 27.86 | |
| ATOM | 2524 | O N | | | | 15.665 | 36.577 | | |
| ATOM | 2525 | N | | C3097 | 17.117 | 17.372 | 35.192 | 1.00 26.91 | И С |
| MOTA | 2526 | CA | | C3097 | 15.874 | 18.045 | 35.521 | 1.00 26.05 | |
| MOTA | 2527 | С | GLY | C3097 | 14.839 | 17.654 | 34.488 | 1.00 25.55 | С |

| ATOM | 2528 | 0 | GLY | C3097 | 15.047 | 16.696 | 33.745 | 1.00 25.35 | 0 |
|-------|------|-----|-----|-------|--------|--------|--------|------------|---|
| ATOM | 2529 | N | LYS | C3098 | 13.729 | 18.384 | 34.428 | 1.00 25.19 | N |
| ATOM | 2530 | CA | LYS | C3098 | 12.690 | 18.086 | 33.452 | 1.00 24.30 | С |
| ATOM | 2531 | CB | LYS | C3098 | 11.320 | 18.543 | 33.945 | 1.00 24.76 | С |
| ATOM | 2532 | CG | | C3098 | 10.863 | 17.934 | 35.237 | 1.00 25.27 | Ċ |
| ATOM | 2533 | CD | | C3098 | 9.397 | 18.241 | 35.459 | 1.00 26.28 | Ċ |
| ATOM | 2534 | CE | | C3098 | 8.973 | 17.880 | 36.860 | 1.00 26.82 | č |
| ATOM | 2535 | NZ | | C3098 | 9.334 | 16.468 | 37.155 | 1.00 28.61 | N |
| | | | | C3098 | | 18.774 | 32.119 | 1.00 23.93 | C |
| ATOM | 2536 | C | | | 12.978 | | | | |
| ATOM | 2537 | 0 | | C3098 | 13.330 | 19.954 | 32.077 | 1.00 23.38 | 0 |
| ATOM | 2538 | N | | C3099 | 12.821 | 18.019 | 31.034 | 1.00 23.34 | N |
| ATOM | 2539 | CA | | C3099 | 13.033 | 18.536 | 29.690 | 1.00 22.75 | C |
| ATOM | 2540 | CB | | C3099 | 13.960 | 17.613 | 28.874 | 1.00 22.58 | C |
| ATOM | 2541 | | | C3099 | 14.345 | 18.292 | 27.558 | 1.00 22.52 | C |
| MOTA | 2542 | | | C3099 | 15.219 | 17.291 | 29.688 | 1.00 22.55 | С |
| MOTA | 2543 | CD1 | | C3099 | 16.199 | 16.357 | 28.985 | 1.00 22.28 | С |
| MOTA | 2544 | С | ILE | C3099 | 11.676 | 18.617 | 28.990 | 1.00 22.48 | С |
| ATOM | 2545 | 0 | ILE | C3099 | 11.054 | 17.591 | 28.699 | 1.00 22.47 | 0 |
| ATOM | 2546 | N | TRP | C3100 | 11.205 | 19.835 | 28.743 | 1.00 21.77 | N |
| ATOM | 2547 | CA | TRP | C3100 | 9.926 | 20.008 | 28.071 | 1.00 20.54 | С |
| ATOM | 2548 | CB | TRP | C3100 | 9.180 | 21.228 | 28.600 | 1.00 19.83 | C |
| MOTA | 2549 | CG | TRP | C3100 | 8.900 | 21.139 | 30.066 | 1.00 19.91 | С |
| MOTA | 2550 | CD2 | TRP | C3100 | 7.806 | 20.455 | 30.694 | 1.00 19.80 | C |
| ATOM | 2551 | CE2 | TRP | C3100 | 7.968 | 20.605 | 32.091 | 1.00 19.84 | С |
| ATOM | 2552 | CE3 | TRP | C3100 | 6.704 | 19.727 | 30.211 | 1.00 19.87 | С |
| MOTA | 2553 | CD1 | TRP | C3100 | 9.660 | 21.660 | 31.081 | 1.00 19.93 | C |
| ATOM | 2554 | NE1 | TRP | C3100 | 9.106 | 21.343 | 32.296 | 1.00 19.91 | N |
| ATOM | 2555 | CZ2 | TRP | C3100 | 7.069 | 20.058 | 33.015 | 1.00 19.27 | С |
| MOTA | 2556 | CZ3 | TRP | C3100 | 5.808 | 19.181 | 31.128 | 1.00 19.78 | С |
| ATOM | 2557 | | | C3100 | 6.000 | 19.352 | 32.520 | 1.00 20.41 | C |
| ATOM | 2558 | Ċ | | C3100 | 10.239 | 20.174 | 26.611 | 1.00 20.42 | C |
| ATOM | 2559 | 0 | | C3100 | 10.831 | 21.174 | 26.195 | 1.00 21.30 | 0 |
| ATOM | 2560 | N | | C3101 | 9.845 | 19.173 | 25.838 | 1.00 19.69 | N |
| ATOM | 2561 | CA | | C3101 | 10.097 | 19.143 | 24.416 | 1.00 19.35 | C |
| ATOM | 2562 | CB | | C3101 | 10.903 | 17.891 | 24.072 | 1.00 18.36 | С |
| ATOM | 2563 | CG | | C3101 | 10.885 | 17.499 | 22.592 | 1.00 18.24 | Ċ |
| ATOM | 2564 | | | C3101 | 11.677 | 18.536 | 21.786 | 1.00 16.55 | C |
| ATOM | 2565 | | | C3101 | 11.466 | 16.097 | 22.414 | 1.00 17.56 | C |
| ATOM | 2566 | c | | C3101 | 8.831 | 19.145 | 23.587 | 1.00 19.41 | Ċ |
| ATOM | 2567 | Ō | | C3101 | 7.846 | 18.493 | 23.929 | 1.00 19.45 | Ö |
| ATOM | 2568 | N | | C3102 | 8.860 | 19.885 | 22.490 | 1.00 19.43 | N |
| ATOM | 2569 | CA | | C3102 | 7.722 | 19.899 | 21.596 | 1.00 19.85 | C |
| ATOM | 2570 | СВ | | C3102 | 6.793 | 21.082 | 21.873 | 1.00 19.85 | Č |
| ATOM | 2571 | OG | | C3102 | | 20.887 | 21.212 | 1.00 19.01 | Ō |
| ATOM | 2572 | C | | C3102 | 8.269 | 19.972 | 20.190 | 1.00 20.13 | c |
| ATOM | 2573 | ō | | C3102 | 9.272 | 20.637 | 19.939 | 1.00 19.67 | Ō |
| ATOM | 2574 | N | | C3103 | 7.624 | 19.251 | 19.282 | 1.00 21.04 | N |
| ATOM | 2575 | CA | | C3103 | 8.037 | 19:231 | 17.889 | 1.00 22.10 | c |
| ATOM | 2576 | CB | | C3103 | 8.735 | 17.906 | 17.523 | 1.00 21.92 | c |
| MOTA | 2577 | | | C3103 | 9.127 | 17.922 | 16.059 | 1.00 21.89 | Č |
| ATOM | 2578 | | | C3103 | 9.963 | 17.681 | 18.405 | 1.00 22.24 | C |
| ATOM | 2579 | | | C3103 | 10.695 | 16.376 | 18.094 | 1.00 22.24 | Č |
| MOTA | 2580 | C | | C3103 | 6.804 | 19.346 | 17.010 | 1.00 23.17 | c |
| MOTA | 2581 | 0 | | C3103 | 5.753 | 18.805 | 17.338 | 1.00 23.17 | 0 |
| ATOM | 2582 | N | | C3103 | 6.932 | 20.051 | 15.896 | 1.00 23.79 | N |
| ATOM | 2583 | CA | | C3104 | 5.829 | 20.031 | 14.965 | 1.00 23.73 | C |
| ATOM | 2584 | CB | | C3104 | 4.989 | 21.419 | 15.294 | 1.00 24.69 | č |
| AI OF | 2004 | CD | UER | 60104 | 4.203 | 21.413 | 13.439 | 1.00 44.03 | C |

| 7.004 | 2525 | 00 | 222 | 00104 | 2 005 | 23 546 | 14.390 | 1 00 1 | 34 65 | , ^ | |
|-------|------|-----|-----|-------|---------|--------|--------|--------|-------|-----|--|
| MOTA | 2585 | OG | | C3104 | 3.905 | 21.546 | | 1.00 2 | | 0 | |
| MOTA | 2586 | С | | C3104 | 6.423 | 20.295 | 13.567 | 1.00 2 | | C | |
| MOTA | 2587 | 0 | SER | C3104 | 7.577 | 20.690 | 13.403 | 1.00 | 25.83 | 0 | |
| ATOM | 2588 | N | HIS | C3105 | 5.646 | 19.929 | 12.560 | 1.00 2 | 27.14 | N | |
| ATOM | 2589 | CA | HIS | C3105 | 6.140 | 19.996 | 11.200 | 1.00 2 | 28.67 | С | |
| MOTA | 2590 | CB | HIS | C3105 | 6.841 | 18.686 | 10.819 | 1.00 | 30.20 | С | |
| ATOM | 2591 | CG | HIS | C3105 | 5.901 | 17.542 | 10.584 | 1.00 | 31.48 | ·C | |
| ATOM | 2592 | | | C3105 | 5.474 | 16.961 | 9.437 | 1.00 | | C | |
| ATOM | 2593 | | | C3105 | 5.252 | 16.887 | 11.607 | 1.00 | | N | |
| ATOM | 2594 | | | C3105 | 4.465 | 15.952 | 11.103 | 1.00 | | C | |
| | | | | | | 15.977 | 9.787 | 1.00 | | | |
| ATOM | 2595 | | | C3105 | 4.580 | | | | | N | |
| MOTA | 2596 | С | | C3105 | 5.046 | 20.253 | 10.187 | 1.00 | | C | |
| MOTA | 2597 | 0 | | C3105 | 3.862 | 20.082 | 10.468 | 1.00 | | 0 | |
| MOTA | 2598 | N | THR | C3106 | 5.478 | 20.682 | 9.009 | 1.00 | | N | |
| ATOM | 2599 | CA | | C3106 | 4.609 | 20.918 | 7.871 | 1.00 | 30.87 | С | |
| MOTA | 2600 | CB | THR | C3106 | 4.542 | 22.416 | 7.492 | 1.00 | 30.95 | С | |
| ATOM | 2601 | OG1 | THR | C3106 | 5.853 | 22.895 | 7.185 | 1.00 | 31.53 | 0 | |
| ATOM | 2602 | CG2 | THR | C3106 | 3.970 | 23.231 | 8.631 | 1.00 | 31.66 | С | |
| ATOM | 2603 | С | THR | C3106 | 5.310 | 20.118 | 6.758 | 1.00 | 31.46 | С | |
| ATOM | 2604 | 0 | | C3106 | 6.288 | 19.411 | 7.032 | 1.00 | | 0 | |
| ATOM | 2605 | N | | C3107 | 4.834 | 20.223 | 5.521 | 1.00 | | N | |
| ATOM | 2606 | CA | | C3107 | 5.444 | 19.475 | 4.423 | 1.00 | | C | |
| ATOM | 2607 | CB | | C3107 | 4.584 | 19.570 | 3.151 | 1.00 | | Ċ | |
| | | | | C3107 | | | 3.276 | 1.00 | | C | |
| ATOM | 2608 | CG | | | 3.252 | 18.836 | | | | | |
| ATOM | 2609 | | | C3107 | 3.059 | 18.077 | 4.257 | 1.00 | | 0 | |
| ATOM | 2610 | | | C3107 | 2.396 | 19.017 | 2.379 | 1.00 | | 0 | |
| ATOM | 2611 | ¢ | | C3107 | 6.861 | 19.942 | 4.096 | 1.00 | | С | |
| MOTA | 2612 | 0 | | C3107 | 7.680 | 19.158 | 3.609 | 1.00 | 32.63 | 0 | |
| MOTA | 2613 | N | GLN | C3108 | 7.152 | 21.210 | 4.371 | 1.00 | 31.99 | N | |
| MOTA | 2614 | CA | GLN | C3108 | 8.467 | 21.768 | 4.068 | 1.00 | 31.59 | С | |
| MOTA | 2615 | CB | GLN | C3108 | 8.310 | 23.119 | 3.362 | 1.00 | 32.00 | С | |
| MOTA | 2616 | CG | GLN | C3108 | 7.482 | 23.077 | 2.086 | 1.00 | 32.40 | , C | |
| ATOM | 2617 | CD | GLN | C3108 | 7.294 | 24.452 | 1.469 | 0.05 | 32.28 | С | |
| ATOM | 2618 | | | C3108 | 6.650 | 24.597 | 0.430 | 0.05 | | 0 | |
| ATOM | 2619 | | | C3108 | 7.856 | 25.469 | 2.110 | 0.05 | | N | |
| ATOM | 2620 | C | | C3108 | 9.391 | 21.957 | 5.272 | 1.00 | | C | |
| ATOM | 2621 | Ö | | C3108 | 10.610 | 21.833 | 5.145 | 1.00 | | Ō | |
| ATOM | 2622 | N | | C3109 | 8.822 | 22.258 | 6.436 | 1.00 | | N | |
| ATOM | 2623 | CA | | C3109 | 9.648 | 22.489 | 7.610 | 1.00 | | C | |
| | | | | C3109 | 9.652 | 23.980 | 7.953 | 1.00 | | c | |
| MOTA | 2624 | CB | | | | | | | | C | |
| ATOM | 2625 | CG | | C3109 | 10.111 | 24.857 | 6.827 | 1.00 | | | |
| ATOM | 2626 | | | C3109 | 9.215 | 25.275 | 5.845 | | 31.09 | C | |
| ATOM | 2627 | | | C3109 | 11.440 | 25.259 | 6.738 | | 30.59 | C | |
| MOTA | 2628 | | | C3109 | 9.636 | 26.084 | 4.788 | | 31.21 | С | |
| MOTA | 2629 | | | C3109 | 11.870 | 26.066 | 5.688 | | 30.89 | C | |
| ATOM | 2630 | CZ | | C3109 | 10.964 | | 4.709 | 1.00 | | С | |
| MOTA | 2631 | С | PHE | C3109 | 9.292 | 21.716 | 8.860 | | 28.01 | C | |
| MOTA | 2632 | 0 | PHE | C3109 | 8.252 | 21:065 | 8.936 | 1.00 | 28.14 | 0 | |
| ATOM | 2633 | N | VAL | C3110 | 10.192 | 21.798 | 9.838 | 1.00 | 26.84 | N | |
| ATOM | 2634 | CA | VAL | C3110 | 10.019 | 21.175 | 11.140 | 1.00 | 25.60 | C | |
| ATOM | 2635 | CB | VAL | C3110 | 10.766 | 19.822 | 11.250 | 1.00 | 25.63 | С | |
| ATOM | 2636 | | | C3110 | 12.268 | 20.035 | 11.191 | | 25.54 | С | |
| ATOM | 2637 | | | C3110 | (10.387 | 19.133 | 12.554 | | 25.58 | C | |
| ATOM | 2638 | C | | C3110 | 10.580 | 22.139 | 12.187 | | 24.84 | C | |
| ATOM | 2639 | 0 | | C3110 | 11.596 | 22.798 | 11.957 | | 24.75 | ō | |
| ATOM | 2640 | N | | C3111 | 9.911 | 22.730 | 13.328 | | 23.62 | N | |
| | | | | | | | | | | C | |
| MOTA | 2641 | CA | THK | C3111 | 10.377 | 23.120 | 14.395 | 1.00 | 23.00 | C | |

| ATOM | 2642 | CB | THR | C3111 | 9.451- | 24.332 | 14.583 | 1.00 23.10 | С |
|------|------|-----|-----|-------|--------|--------|--------|------------|-----|
| ATOM | 2643 | OG1 | THR | C3111 | 8.138 | 23.871 | 14.924 | 1.00 24.21 | 0 |
| MOTA | 2644 | CG2 | THR | C3111 | 9.369 | 25.145 | 13.306 | 1.00 23.43 | С |
| ATOM | 2645 | С | | C3111 | 10.424 | 22.363 | 15.712 | 1.00 22.01 | С |
| ATOM | 2646 | 0 | | C3111 | 9.616 | 21.466 | 15.951 | 1.00 22.10 | 0 |
| ATOM | 2647 | N | | C3112 | 11.382 | 22.726 | 16.554 | 1.00 21.05 | |
| ATOM | 2648 | CA | | C3112 | 11.532 | 22.110 | 17.859 | 1.00 20.79 | |
| ATOM | 2649 | CB | | C3112 | 12.710 | 21.135 | 17.846 | 1.00 20.00 | |
| ATOM | 2650 | C | | C3112 | 11.741 | 23.194 | 18.927 | 1.00 20.81 | |
| ATOM | 2651 | 0 | | C3112 | 12.367 | 24.216 | 18.672 | 1.00 20.76 | |
| | 2652 | N | | C3112 | 11.199 | 22.968 | 20.118 | 1.00 20.70 | |
| ATOM | | | | C3113 | 11.346 | 23.909 | 21.215 | 1.00 20.61 | |
| ATOM | 2653 | CA | | C3113 | 10.061 | | 21.213 | 1.00 20.01 | |
| ATOM | 2654 | CB | | | | 24.721 | | | |
| ATOM | 2655 | OG | | C3113 | 10.176 | 25.598 | 22.526 | 1.00 20.34 | |
| ATOM | 2656 | C | | C3113 | 11.653 | 23.128 | 22.477 | 1.00 20.63 | |
| ATOM | 2657 | 0 | | C3113 | 11.013 | 22.119 | 22.759 | 1.00 20.86 | |
| ATOM | 2658 | N | | C3114 | 12.633 | 23.599 | 23.237 | 1.00 20.54 | |
| ATOM | 2659 | CA | | C3114 | 13.019 | 22.938 | 24.463 | 1.00 20.40 | |
| MOTA | 2660 | CB | | C3114 | 14.349 | 22.188 | 24.288 | 1.00 20.41 | |
| ATOM | 2661 | | | C3114 | 14.872 | 21.743 | 25.647 | 1.00 19.44 | |
| MOTA | 2662 | CG2 | | C3114 | 14.143 | 20.976 | 23.357 | 1.00 20.11 | |
| ATOM | 2663 | С | | C3114 | 13.159 | 23.883 | 25.644 | 1.00 20.99 | |
| MOTA | 2664 | 0 | VAL | C3114 | 13.804 | 24.938 | 25.552 | 1.00 20.99 | |
| MOTA | 2665 | N | ILE | C3115 | 12.543 | 23,494 | 26.756 | 1.00 21.35 | |
| MOTA | 2666 | CA | ILE | C3115 | 12.626 | 24.269 | 27.980 | 1.00 22.44 | |
| MOTA | 2667 | CB | ILE | C3115 | 11.250 | 24.816 | 28.428 | 1.00 22.27 | |
| ATOM | 2668 | CG2 | ILE | C3115 | 11.440 | 25.821 | 29.562 | 1.00 22.27 | |
| ATOM | 2669 | CG1 | ILE | C3115 | 10.553 | 25.529 | 27.262 | 1.00 22.90 | |
| ATOM | 2670 | CD1 | ILE | C3115 | 9.141 | 25.990 | 27.582 | 1.00 22.49 | C |
| MOTA | 2671 | С | ILE | C3115 | 13.167 | 23.360 | 29.077 | 1.00 23.09 | C |
| ATOM | 2672 | 0 | ILE | C3115 | 12.570 | 22.331 | 29.388 | 1.00 23.11 | . 0 |
| ATOM | 2673 | N | LEU | C3116 | 14.311 | 23.730 | 29.640 | 1.00 23.90 | N |
| ATOM | 2674 | CA | LEU | C3116 | 14.912 | 22.959 | 30.720 | 1.00 25.63 | C |
| ATOM | 2675 | CB | LEU | C3116 | 16.434 | 23.051 | 30.667 | 1.00 24.96 | G C |
| ATOM | 2676 | CG | LEU | C3116 | 17.007 | 22.497 | 29.366 | 1.00 24.50 |) C |
| ATOM | 2677 | CD1 | LEU | C3116 | 18.508 | 22.663 | 29.350 | 1.00 23.62 | . C |
| ATOM | 2678 | | | C3116 | 16.596 | 21.029 | 29.236 | 1.00 24.58 | 3 C |
| MOTA | 2679 | С | | C3116 | 14.418 | 23.524 | 32.036 | 1.00 27.20 |) C |
| ATOM | 2680 | 0 | | C3116 | 14.412 | 24.743 | 32.236 | 1.00 27.34 | |
| ATOM | 2681 | N | | C3117 | 13.998 | 22.636 | 32.930 | 1.00 28.70 | |
| ATOM | 2682 | CA | | C3117 | 13.490 | 23.061 | 34.226 | 1.00 30.61 | |
| MOTA | 2683 | CB | | C3117 | 11.957 | 22.951 | 34.249 | 1.00 30.11 | |
| ATOM | 2684 | CG | | C3117 | 11.322 | 23.257 | 35.592 | 1.00 30.29 | |
| ATOM | 2685 | CD | | C3117 | 9.808 | 23.100 | 35.585 | 1.00 30.63 | |
| ATOM | 2686 | | | C3117 | 9.313 | 22.085 | 35.043 | 1.00 30.65 | |
| ATOM | 2687 | | | C3117 | | | | 1.00 30.59 | |
| ATOM | 2688 | C | | C3117 | 14.089 | 22.241 | 35.357 | 1.00 31.98 | |
| ATOM | 2689 | Ö | | C3117 | 14.353 | 21:052 | 35.205 | 1.00 32.46 | |
| ATOM | 2690 | N | | C3118 | 14.321 | 22.900 | 36.485 | 1.00 33.79 | |
| ATOM | 2691 | CA | | C3118 | 14.863 | 22.257 | 37.674 | 1.00 35.43 | |
| ATOM | 2692 | CB | | C3118 | 16.264 | 22.779 | 37.990 | | |
| ATOM | 2693 | CG | | C3118 | 17.396 | 21.983 | 37.366 | 1.00 38.74 | |
| ATOM | 2694 | CD | | C3118 | 17.335 | 20.507 | 37.733 | 1.00 40.59 | |
| ATOM | 2695 | | | C3118 | 16.936 | 20.189 | 38.881 | 1.00 41.3 | |
| MOTA | 2695 | | | C3118 | 17.700 | 19.669 | 36.877 | 1.00 41.3 | |
| MOTA | 2697 | C | | C3118 | 13.940 | 22.578 | 38.837 | 1.00 36.13 | |
| | | | | | | | | 1.00 30.1 | |
| ATOM | 2698 | 0 | GEO | C3118 | 13.351 | 21.632 | 39.403 | 1.00 37.13 | , 0 |

| ATOM | 2699 | OXT | GLU | C31 | 18 | 13.813 | 23.778 | 39.156 | 1.00 | 36.00 | 0 |
|------|------|-----|-----|------|------------|---------|---------|--------|------|---------|---|
| TER | 2700 | | GLU | | | • | | | | | |
| ATOM | 2701 | 0 | нон | | 1 | 8.576 | 28.003 | 19.046 | | 26.06 | 0 |
| ATOM | 2702 | Ö | нон | | 2 | 11.001 | 13.668 | 14.737 | 1.00 | 16.99 | 0 |
| ATOM | 2703 | ō | НОН | | 3 | -5.347 | 33.382 | 14.724 | 1.00 | 27.55 | 0 |
| ATOM | 2704 | Ō | НОН | | 4 | 19.615 | 31.388 | 19.825 | 1.00 | 18.58 | 0 |
| ATOM | 2705 | 0 | нон | | 5 | -11.216 | 36.113 | 18.617 | 1.00 | 38.18 | 0 |
| | 2706 | 0 | нон | | 6 | 0.159 | 37,746 | 18.293 | | 26.61 | 0 |
| ATOM | | | нон | | 7 | 1.276 | 36.190 | 20.543 | | 28.54 | 0 |
| ATOM | 2707 | 0 | НОН | | 8 | 12.334 | 34.067 | 2.484 | | 24.27 | 0 |
| ATOM | 2708 | 0 | НОН | | 9 | 0.255 | 6.277 | 33.704 | | 25.24 | 0 |
| ATOM | 2709 | 0 | | | 10 | 18.182 | 37.167 | 27.027 | | 23.05 | 0 |
| MOTA | 2710 | 0 | HOH | | 11 | -4.577 | 31.410 | 31.511 | | 38.36 | 0 |
| ATOM | 2711 | 0 | HOH | | | -1.511 | 45.557 | 32.920 | | 53.67 | 0 |
| MOTA | 2712 | 0 | HOH | | 12 | 18.448 | 25.653 | 12.095 | | 26.48 | 0 |
| ATOM | 2713 | 0 | НОН | | 13 | 3.912 | 2.648 | 29.570 | | 20.27 | 0 |
| MOTA | 2714 | 0 | HOH | | 14 | -11.595 | 44.974 | 29.760 | | 29.90 | 0 |
| MOTA | 2715 | 0 | НОН | | 15 | | 18.367 | 31.463 | | 31.92 | 0 |
| ATOM | 2716 | 0 | НОН | | 16 | 25.183 | 28.443 | 2.735 | | 24.74 | Ō |
| ATOM | 2717 | 0 | нон | | 17 | 1.272 | | 7.542 | | 32.28 | Ö |
| MOTA | 2718 | 0 | нон | | 18 | 19.674 | 51.864 | | | 37.76 | ŏ |
| MOTA | 2719 | 0 | HOH | | 19 | 7.406 | 44.679 | 0.671 | | 37.75 | Ö |
| MOTA | 2720 | 0 | нон | W | 20 | 9.102 | 25.639 | 41.587 | | | Ö |
| ATOM | 2721 | 0 | нон | | 21 | -2.117 | 42.358 | 29.367 | | 23.51 | Ö |
| MOTA | 2722 | 0 | нон | | 22 | 12.144 | 15.091 | 31.453 | | 40.21 | 0 |
| ATOM | 2723 | 0 | HOH | W | 23 | 20.216 | 37.895 | 14.318 | | 23.27 | 0 |
| MOTA | 2724 | 0 | нон | W | 24 | 15.409 | 30.644 | 36.448 | | 34.67 | 0 |
| ATOM | 2725 | 0 | НОН | W | 25 | 8.888 | 28.186 | 21.855 | | 19.15 | |
| MOTA | 2726 | 0 | HOH | W | 26 | -6.604 | 42.281 | 29.309 | | 52.83 | 0 |
| ATOM | 2727 | 0 | нон | W | 27 | 20.104 | 53.238 | 15.360 | | 42.16 | 0 |
| ATOM | 2728 | 0 | НОН | W | 28 | 24.519 | 36.311 | 10.567 | | 45.76 | 0 |
| MOTA | 2729 | 0 | нон | W | 29 | 17.712 | 23.831 | 7.356 | | 49.27 | 0 |
| MOTA | 2730 | 0 | НОН | W | 30 | -6.885 | 28.651 | 32.939 | | 45.10 | 0 |
| ATOM | 2731 | 0 | HOH | W | 31 | -4.869 | 16.926 | 12.390 | | 39.22 | 0 |
| ATOM | 2732 | 0 | HOH | W | 32 | 20.935 | 28.085 | 34.073 | | 42.57 | 0 |
| MOTA | 2733 | 0 | HOH | I W | 33 | 21.868 | 15.456 | 38.834 | | 28.55 | 0 |
| ATOM | 2734 | 0 | HOH | W | 34 | 30.171 | 27.602 | 20.593 | | 34.40 | 0 |
| MOTA | 2735 | 0 | HOF | W | 35 | 20.651 | 33.038 | 6.426 | | 38.43 | 0 |
| ATOM | 2736 | 0 | HOH | I W | 36 | 10.238 | 19.208 | 1.078 | | 45.56 | 0 |
| MOTA | 2737 | 0 | HOH | W I | 37 | 13.283 | 54.499 | 28.613 | | 29.72 | 0 |
| ATOM | 2738 | 0 | HOH | I W | 38 | -11.211 | 32.999 | 2.256 | | 31.79 | 0 |
| ATOM | 2739 | 0 | HOI | ł W | 3 9 | 9.887 | 29.798 | 36.670 | | 39.85 | 0 |
| ATOM | 2740 | 0 | HOI | ł W. | 40 | 18.546 | 10.765 | 31.009 | | 38.20 | 0 |
| MOTA | 2741 | 0 | нон | W F | 41 | 24.510 | 24.190 | 30.902 | | 36.49 | 0 |
| ATOM | 2742 | 0 | HOI | H W | 42 | 30.384 | 38.300 | 20.406 | | 44.88 | 0 |
| ATOM | 2743 | 0 | | H W | 43 | 18.885 | 28.685 | 22,975 | | 28.61 | 0 |
| ATOM | 2744 | | HO | H W | 44 | 2.917 | 33.308 | 36.961 | | 38.63 | 0 |
| ATOM | 2745 | | | H W | 45 | 20.025 | | 29.500 | | 35.61 | 0 |
| ATOM | 2746 | | | H W | 46 | 8.253 | 16:151 | 27.102 | | 0 45.55 | 0 |
| ATOM | 2747 | | | H W | 47 | 7.572 | 21.032 | 36.495 | | 0 16.73 | 0 |
| ATOM | 2748 | | | H W | 48 | 19.451 | | 27.413 | 1.0 | 0 35.89 | 0 |
| MOTA | 2749 | | | H W | 49 | 11.476 | | 36.574 | | 0 25.09 | 0 |
| ATOM | 2750 | | | H W | | 14.236 | | | | 0 34.47 | 0 |
| ATOM | 2751 | | | H W | | 5.103 | | | | 0 41.40 | 0 |
| ATOM | 2752 | | | H W | | 34.054 | | | 1.0 | 0 45.36 | 0 |
| MOTA | 2753 | | | H W | | 12.068 | | | 1.0 | 0 39.74 | 0 |
| ATOM | 2754 | | | H W | | 2.919 | | | | 0 41.17 | 0 |
| | 2755 | | | H W | | 27.605 | | | | 0 50.62 | 0 |
| ATOM | 213 | | | ** | | | | | | | |

| ATOM | 2756 | 0 | нон w | 56 | -12.868 | | 30.495 | 1.00 | | 0 |
|--------------|--------------|-----|-------|-------------|-------------------|------------------|------------------|------|--------------------|---|
| ATOM | 2757 | 0 | HOH W | 57 | 9.027 | | 36.816 | 1.00 | | 0 |
| ATOM | 2758 | 0 | HOH W | 58 | 7.507 | 37.992 | 7.686 | 1.00 | | 0 |
| MOTA | 2759 | 0 | HOH W | 59 | 18.024 | 26.076 | 4.943 | | 45.92 | 0 |
| MOTA | 2760 | 0 | HOH W | 60 | 21.889 | 53.044 | 19.501 | | 41.90 | 0 |
| MOTA | 2761 | 0 | HOH W | 61 | 34.566 | 32.372 | 30.692 | | 50.00 | 0 |
| ATOM | 2762 | 0 | HOH W | 62 | 5.289 | 23.268 | 4.539 | | 26.10 | 0 |
| MOTA | 2763 | 0 | HOH W | 63 | 21.724 | 28.905 | 29.036 | | 54.44 | 0 |
| MOTA | 2764 | 0 | НОН M | 64 | 7.000 | 28.471 | 37.399 | | 36.37 | 0 |
| MOTA | 2765 | 0 | HOH W | 65 | 31.382 | 30.725 | 21.632 | | 32.29 | 0 |
| ATOM | 2766 | 0 | HOH W | 66 | 28.182 | 46.827 | 4.332 | | 48.39 | 0 |
| MOTA | 2767 | 0 | HOH W | 67 | 7.410 | 9.794 | 14.247 | | 49.84 43.26 | Ö |
| MOTA | 2768 | 0 | HOH W | 68 | 31.517 | 25.424 | 22.117 | | 34.98 | ŏ |
| ATOM | 2769 | 0 | HOH W | 69 | -5.301 | 33.373 | 34.239 30.281 | | 41.21 | ŏ |
| MOTA | 2770 | 0 | HOH W | 70 | 36.871 | 33.074 | 17.966 | | 33.98 | Ö |
| MOTA | 2771 | 0 | HOH W | 71 | 24.903 | 41.702 | 31.211 | | 35.46 | Ö |
| MOTA | 2772 | 0 | HOH W | 72 | 17.963 | 38.386 | 4.797 | | 50.12 | ō |
| ATOM | 2773 | 0 | HOH W | 73 | 20.723 | 48.845 30.159 | 31.227 | | 58.73 | ō |
| ATOM | 2774 | 0 | HOH W | 74 | -8.379 | | 10.013 | | 53.09 | Ö |
| MOTA | 2775 | 0 | HOH W | 75 76 | -1.343 | 19.609 12.801 | 31.165 | | 65.31 | Ö |
| ATOM | 2776 | 0 | HOH W | 76 | 15.642 -14.605 | 25.461 | 6.171 | | 36.87 | 0 |
| MOTA | 2777 | 0 | HOH W | 77 78 | 8.718 | 39.594 | 0.632 | | 44.46 | 0 |
| ATOM | 2778 | 0 | HOH W | 78 79 | 22.426 | 26.766 | 11.895 | | 39.57 | O |
| MOTA | 2779 | 0 | HOH W | 80 | 1.403 | 12.128 | 29.940 | | 41.04 | 0 |
| ATOM | 2780 | 0 | HOH W | 81 | 9.724 | 26.576 | 37.441 | | 52.28 | 0 |
| ATOM | 2781 | 0 | HOH W | 82 | -20.852 | 35.093 | 18.162 | | 32.23 | 0 |
| ATOM | 2782 | 0 | HOH W | | -22.727 | 33.513 | 17.160 | | 46.00 | 0 |
| MOTA | 2783 | 0 | HOH W | | -9.764 | 38.910 | 4.301 | | 38.92 | 0 |
| ATOM | 2784 | 0 | HOH W | | 4.067 | 40.345 | 32.364 | | 54.10 | 0 |
| ATOM | 2785 | 0 | HOH W | | 8.783 | 44.044 | 3.423 | | 45.06 | 0 |
| ATOM | 2786 2787 | 0 | HOH W | | 19.259 | 34.587 | 26.113 | | 34.60 | 0 |
| MOTA | 2788 | 0 | HOH W | | 19.168 | 34.051 | 31.232 | | 40.61 | 0 |
| MOTA | 2789 | 0 | HOH W | | -17.637 | 26.480 | 8.650 | 1.00 | 35.76 | 0 |
| MOTA MOTA | 2790 | 0 | HOH W | | 5.883 | 33.114 | 4.115 | | 36.72 | 0 |
| ATOM | 2791 | ŏ | HOH W | | 5.401 | 9.271 | 3.439 | 1.00 | 23.12 | 0 |
| ATOM | 2792 | Ö | HOH W | | 16.578 | 55.625 | 9.782 | 1.00 | 34.03 | 0 |
| ATOM | 2793 | Ö | нон м | | -6.649 | 22.603 | 36.177 | | 49.27 | 0 |
| ATOM | 2794 | ō | HOH W | | 12.263 | 32.477 | 39.013 | | 44.31 | 0 |
| ATOM | 2795 | ō | нон м | | 11.064 | 51.183 | 10.359 | | 46.81 | 0 |
| ATOM | 2796 | 0 | HOH W | 96 | -16.103 | 28.570 | 5.999 | | 45.48 | 0 |
| ATOM | 2797 | 0 | HOH W | v 97 | 19.096 | 56.580 | 8.669 | | 48.52 | 0 |
| MOTA | 2798 | 0 | HOH V | v 98 | -0.441 | 38.083 | 25.842 | | 30.49 | 0 |
| MOTA | 2799 | 0 | нон и | | 18.821 | 50.159 | 23.847 | | 35.93 | 0 |
| ATOM | 2800 | 0 | HOH V | v 100 | 21.593 | | 22.517 | 1.00 | 46.08 | 0 |
| MOTA | 2801 | 0 | | v 101 | 24.154 | 31.033 | 26.613 | | 41.03 | 0 |
| ATOM | 2802 | 0 | HOH V | N 102 | 18.634 | 43.303 | 30.404 | | 40.85 | |
| ATOM | 2803 | 0 | | N 103 | 19.981 | 32.247 | 35.107 | | 36.43 | 0 |
| MOTA | 2804 | 0 | | N 104 | -10.088 | | 1.003 | | 36.43 | 0 |
| MOTA | 2805 | 0 | | W 105 | -18.529 | | 5.334 | | 38.77 | Ö |
| MOTA | 2806 | | | W 106 | -20.984 | | 15.095 | | 0 40.22 | 0 |
| ATOM | 2807 | | | W 107 | -19.013 | | | | 32.06 | 0 |
| MOTA | 2808 | | | W 108 | -14.266 | | | | 0 41.92 | 0 |
| MOTA | 2809 | | | W 109 | 7.301 | | | | 0 37.73 0 37.13 | 0 |
| ATOM | 2810 | | | W 110 | 24.398 | | | | 0 37.13 | Ö |
| MOTA | 2811 | | | W 111 | 2.259 | | | | 0 46.84 | o |
| MOTA | 2812 | 2 0 | нон | W 112 | 22.143 | 19.952 | 3.110 | 1.0 | J 30.03 | _ |

| | | | | | | | • | |
|------|------|---|-----------|--------|--------|--------|------------|-----|
| ATOM | 2813 | 0 | HOH W 113 | -4.490 | 20.867 | 8.897 | 1.00 50.63 | 0 |
| ATOM | 2814 | 0 | HOH W 114 | 0.274 | 4.462 | 29.620 | 1.00 46.55 | 0 |
| MOTA | 2815 | 0 | HOH W 115 | 9.966 | 5.205 | 19.879 | 1.00 29.38 | 0 |
| ATOM | 2816 | 0 | HOH W 116 | 11.609 | 14.420 | 39.214 | 1.00 45.17 | 0 |
| ATOM | 2817 | 0 | HOH W 117 | 21.720 | 11.206 | 36.139 | 1.00 23.23 | Ō |
| ATOM | 2818 | 0 | HOH W 118 | 21.825 | 46.932 | 3.417 | 1.00 42.90 | 0 |
| MOTA | 2819 | 0 | HOH W 119 | 0.067 | 30.700 | 1.199 | 1.00 54.52 | 0 |
| ATOM | 2820 | 0 | HOH W 120 | 10.218 | 22.583 | 38.806 | 1.00 43.46 | 0 |
| MOTA | 2821 | 0 | HOH W 121 | 0.686 | 27.966 | 42.608 | 1.00 42.57 | 0 |
| ATOM | 2822 | 0 | HOH W 122 | 23.786 | 35.976 | 16.687 | 1.00 27.98 | 0 |
| MOTA | 2823 | 0 | HOH W 123 | 25.685 | 36.926 | 14.983 | 1.00 35.19 | 0 |
| ATOM | 2824 | 0 | HOH W 124 | 5.593 | 17.615 | 20.205 | 1.00 22.22 | 0 |
| ATOM | 2825 | 0 | HOH W 125 | -3.621 | 36.444 | 16.059 | 1.00 38.53 | 0 |
| MOTA | 2826 | 0 | HOH W 126 | -6.822 | 38.370 | 14.785 | 1.00 35.77 | . 0 |
| MOTA | 2827 | 0 | HOH W 127 | 8.658 | 28.063 | 15.129 | 1.00 32.14 | 0 |
| MOTA | 2828 | 0 | HOH W 128 | -4.302 | 30.987 | 36.514 | 1.00 38.06 | 0 |
| ATOM | 2829 | 0 | HOH W 129 | -1.650 | 29.068 | 38.757 | 1.00 30.65 | 0 |
| TER | 2830 | | HOH W 129 | | | | | |
| END | | | • | | | | | |
| | | | | | | | | |

TABLE 4

```
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 2.05 A
REMARK starting r= 0.2078 free_r= 0.2459
REMARK final r= 0.2076 free r= 0.2466
REMARK B rmsd for bonded mainchain atoms= 1.338 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.017 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.137 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.077 target= 2.5
REMARK wa= 1.98578
REMARK rweight=0.12477
REMARK target= mlf · steps= 30
REMARK sg= C2 a= 116.043 b= 59.291 c= 49.629 alpha= 90 beta= 98.768 gamma= 90
REMARK parameter file 1 : CNX_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNX_TOPPAR:water_rep.param
REMARK parameter file 3 : CNX_TOPPAR:ion.param
REMARK molecular structure file: generate.psf
REMARK input coordinates: minimize.pdb
REMARK reflection file= ../data/x-ray_data.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 2.05
REMARK initial B-factor correction applied to fobs :
REMARK B11= 0.091 B22= -2.051 B33= 1.959
REMARK B12= 0.000 B13= 0.271 B23= 0.000
REMARK B-factor correction applied to coordinate array B: -0.022
REMARK bulk solvent: (Mask) density level= 0.368883 e/A^3, B-factor= 52.2583 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range:
                                                                                     21048 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):
                                                                                    1611 ( 7.7 %)
                                                                                       0 (
                                                                                                0.0 %)
REMARK number of reflections rejected:
                                                                                     19437 ( 92.3 % )
REMARK total number of reflections used:
REMARK number of reflections in working set:
                                                                                     18494 ( 87.9 % )
                                                                                       943 (
                                                                                                 4.5 %)
REMARK number of reflections in test set:
REMARK FILENAME="acps native 2.pdb"
                                                      created by user: rx83663
REMARK Written by CNX VERSION: 2000
ATOM 1 CB MET A1003
ATOM 2 CG MET A1003
ATOM 3 SD MET A1003
                                                      5.413 19.351 .1.00 32.48
5.856 20.649 1.00 37.79
                                                                                                         С
                                            36.109
                                            35.473
                                                        6.848 21.649 1.00 45.89
                                            36.607
             4 CE MET A1003
                                                        8.314 20.599 1.00 43.10
                                                                                                         С
                                            36.791
MOTA
           5 C MET A1003
6 O MET A1003
7 N MET A1003
8 CA MET A1003
9 N ILE A1004
                                                                                                         С
                                            33.900 5.073 18.225 1.00 27.65
ATOM
                                           33.795 6.027 17.463 1.00 25.93
35.971 4.133 17.240 1.00 28.87
35.262 4.452 18.515 1.00 29.37
32.860 4.513 18.832 1.00 27.12
31.500 5.005 18.649 1.00 25.95
                                                                                                         0
MOTA
                                                                                                         N
MOTA
                                                                                                         С
MOTA
                                                                                                         N
            9 N ILE A1004
10 CA ILE A1004
11 CB ILE A1004
MOTA
                                                                                                         С
MOTA
                                            30.463 .3.928 19.020 1.00 25.43
MOTA
                                                                                                         С
            12 CG2 ILE A1004
                                           29.048 4.516 18.954 1.00 24.89
MOTA
                                           30.604 2.730 18.076 1.00 24.55
                                                                                                         C
           13 CG1 ILE A1004
ATOM

    29.619
    1.616
    18.347
    1.00
    26.14

    31.289
    6.214
    19.546
    1.00
    27.18

    31.700
    6.212
    20.703
    1.00
    27.39

    30.655
    7.251
    19.018
    1.00
    24.87

    30.420
    8.439
    19.818
    1.00
    25.40

           14 CD1 ILE A1004
MOTA
           15 C
                       ILE A1004
MOTA
           16 O ILE A1004 31.700 6.212 20.703 1.00 27.39 17 N VAL A1005 30.655 7.251 19.018 1.00 24.87 18 CA VAL A1005 30.420 8.439 19.818 1.00 25.40 19 CB VAL A1005 31.326 9.589 19.346 1.00 26.42 20 CG1 VAL A1005 32.781 9.240 19.648 1.00 26.20 21 CG2 VAL A1005 31.153 9.818 17.860 1.00 27.65
MOTA
MOTA
 MOTA
                                                                                                         C
 ATOM
                                                                                                         С
 ATOM
 ATOM
```

| ATOM | 22 | С | VAL | A1005 | 28.955 | 8.857 | 19.794 | 1.00 | 24.30 | С |
|--------------|------------|----------|-----|----------------|------------------|----------------|------------------|------|-------------|---|
| ATOM | 23 | 0 | VAL | A1005 | 28.592 | 9.964 | 20.195 | 1.00 | 23.88 | 0 |
| ATOM | 24 | N | GLY | A1006 | 28.102 | 7.952 | 19.331 | 1.00 | 23.00 | N |
| ATOM | 25 | CA | GLY | A1006 | 26.687 | 8.261 | 19.290 | 1.00 | 19.45 | С |
| ATOM | 26 | С | GLY | A1006 | 25.887 | 7.300 | 18.443 | 1.00 | 18.59 | С |
| MOTA | 27 | 0 | GLY | A1006 | 26.396 | 6.730 | 17.480 | 1.00 | 16.47 | 0 |
| ATOM | 28 | N | HIS | A1007 | 24.621 | 7.130 | 18.809 | 1.00 | 16.39 | N |
| MOTA | 29 | CA | HIS | A1007 | 23.720 | 6.249 | 18.092 | 1.00 | 15.38 | С |
| ATOM | 30 | CB | HIS | A1007 | 23.825 | 4.818 | 18.636 | 1.00 | | С |
| MOTA | 31 | CG | HIS | A1007 | 22.877 | 3.853 | 17.993 | 1.00 | 18.41 | С |
| MOTA | 32 | CD2 | HIS | A1007 | 22.075 | 2.902 | 18.528 | 1.00 | 17.85 | С |
| ATOM | 33 | ND1 | HIS | A1007 | 22.690 | 3.789 | 16.628 | 1.00 | 17.93 | N |
| ATOM | 34 | CE1 | HIS | A1007 | 21.811 | 2.841 | 16.351 | 1.00 | 19.72 | С |
| ATOM | 35 | NE2 | HIS | A1007 | 21.423 | 2.288 | 17.486 | | 18.78 | N |
| MOTA | 36 | С | HIS | A1007 | 22.302 | 6.768 | 18.262 | 1.00 | 16.54 | С |
| ATOM | 37 | 0 | HIS | A1007 | 21.883 | 7.113 | 19.364 | 1.00 | 15.23 | 0 |
| MOTA | 38 | N | GLY | A1008 | 21.568 | 6.844 | 17.162 | | 13.65 | N |
| ATOM | 39 | CA | GLY | A1008 | 20.204 | 7.303 | 17.250 | 1.00 | 14.59 | С |
| ATOM | 40 | С | GLY | A1008 | 19.364 | 6.591 | 16.220 | | 16.81 | С |
| MOTA | 41 | 0 | GLY | A1008 | 19.864 | 6.208 | 15.154 | | 14.95 | 0 |
| ATOM | 42 | N | ILE | A1009 | 18.089 | 6.394 | 16.538 | | 16.05 | N |
| MOTA | 43 | CA | | A1009 | 17.186 | 5.750 | 15.603 | | 16.53 | С |
| MOTA | 44 | CB | ILE | A1009 | 16.841 | 4.297 | 16.012 | | 16.37 | С |
| MOTA | 45 | | | A1009 | 18.087 | 3.436 | 15.974 | | 15.97 | C |
| MOTA | 46 | | | A1009. | 16.168 | 4.284 | 17.393 | | 14.54 | C |
| ATOM | 47 | | | A1009 | 15.697 | 2.907 | 17.831 | | 15.26 | C |
| MOTA | 48 | С | | A1009 | 15.898 | 6.541 | 15.578 | | 18.21 | C |
| ATOM | 49 | . 0 | | A1009 | 15.681 | 7.423 | 16.408 | | 18.91 | 0 |
| MOTA | 50 | N | | A1010 | 15.041 | 6.218 | 14.623 | | 19.48 | N |
| ATOM | 51 | CA | | A1010 | 13.759 | 6.880 | 14.520 | | 20.47 | C |
| ATOM | 52 | CB | | A1010 | 13.930 | 8.295 | 13.969 | | 21.20 | C |
| ATOM | 53 | CG | | A1010 | 12.614 | 9.013 | 13.813 | | 24.68 | C |
| ATOM | 54 | | | A1010 | 12.002 | 8.901 | 12.725 | | 25.58 | 0 |
| ATOM | 55 | | | A1010 | 12.182 | 9.675 | 14.785 | | 21.51 22.13 | C |
| ATOM | 56 | C | | A1010 | 12.822 | 6.094 | 13.630 | | | 0 |
| ATOM | 57 | 0 | | A1010 | 13.249 11.548 | 5.485 6.074 | 12.641 14.011 | | 21.63 | N |
| ATOM | 58 50 | N C2 | | A1011 A1011 | 10.525 | 5.403 | 13.226 | | 22.73 | C |
| ATOM ATOM | 59 60 | CA CB | | A1011 | 10.019 | 4.103 | 13.903 | | 22.88 | č |
| ATOM | 61 | | | A1011 | 9.505 | 4.398 | 15.320 | | 23.25 | č |
| ATOM | 62 | | | A1011 | 8.922 | 3.476 | 13.033 | | 24.40 | Ċ |
| ATOM | 63 | | | A1011 | 8.496 | 2.096 | 13.466 | | 25.25 | Ċ |
| ATOM | 64 | C | | A1011 | 9.394 | 6.412 | 13.094 | | 23.63 | C |
| ATOM | 65 | Ö | | A1011 | 9.016 | 7.061 | 14.071 | | 23.36 | 0 |
| ATOM | 66 | N | | A1012 | 8.869 | 6.549 | 11.882 | | 25.11 | N |
| ATOM | 67 | CA | | A1012 | 7.810 | 7.514 | 11.602 | | 24.91 | С |
| ATOM | 68 | CB | | A1012 | 8.421 | -8.737 | 10.916 | | 25.40 | С |
| ATOM | 69 | CG | | A1012 | 7.413 | 9.773 | 10.433 | | 29.98 | С |
| ATOM | 70 | CD | | A1012 | 6.857 | 10.631 | 11.552 | | 32.43 | C |
| ATOM | 71 | | | A1012 | 5.954 | 11.447 | 11.274 | | 36.73 | 0 |
| ATOM | 72 | | | A1012 | 7.319 | 10.497 | 12.704 | | 35.01 | 0 |
| ATOM | 73 | С | | A1012 | 6.705 | 6.952 | 10.716 | | 24.25 | С |
| ATOM | 74 | 0 | | A1012 | 6.975 | 6.186 | 9.789 | 1.00 | 22.71 | 0 |
| ATOM | 75 | N | | A1013 | 5.462 | 7.331 | 11.006 | 1.00 | 24.75 | N |
| MOTA | 76 | CA | GLU | A1013 | 4.326 | 6.895 | 10.195 | 1.00 | 25.26 | С |
| MOTA | 7 7 | CB | GLU | A1013 | 3.006 | 7.010 | 10.956 | | 27.28 | С |
| MOTA | 78 | CG | GLU | A1013 | 2.782 | 6.015 | 12.056 | 1.00 | 32.89 | С |
| | | | | | | | | | | |

| ATOM | 79 | CD | GLU | A1013 | 1.337 | 6.025 | 12.512 | 1.00 36.18 | C |
|--------------|------------|----------|------|----------------|----------------|------------------|----------------|--------------------------|--------|
| ATOM | 80 | OE1 | GLU | A1013 | 0.451 | 5.792 | 11.661 | 1.00 38.66 | 0 |
| ATOM | 81 | OE2 | GLU | A1013 | 1.083 | 6.270 | 13.709 | 1.00 39.09 | 0 |
| MOTA | 82 | | | A1013 | 4.253 | 7.848 | 9.013 | 1.00 24.28 | C |
| ATOM | 83 | 0 | | A1013 | 4.254 | 9.062 | 9.197 | 1.00 24.07 | 0 |
| ATOM | 84 | N | LEU | A1014 | 4.179 | 7.308 | 7.805 | 1.00 23.86 | N |
| MOTA | 85 | CA | LEU | A1014 | 4.103 | 8.149 | 6.615 | 1.00, 24.45 | C |
| ATOM | 86 | CB | LEU | A1014 | 4.150 | 7.274 | 5.362 | 1.00 25.54 | C |
| ATOM | 87 | CG | | A1014 | 5.402 | 6.397 | 5.287 | 1.00 28.12 | C |
| MOTA | 88 | | | A1014 | 5.266 | 5.386 | 4.162 | 1.00 28.37 | C |
| MOTA | 89 | CD2 | | A1014 | 6.627 | 7.284 | 5.082 | 1.00 29.49 | c |
| ATOM | 90 | С | | A1014 | 2.838 | 9.010 | 6.611 | 1.00 23.06 | C |
| ATOM | 91 | 0 | | A1014 | 2.838 | 10.126 | 6.083 | 1.00 22.31 | 0 |
| ATOM | 92 | N | | A1015 | 1.768 | 8.490 | 7.210 | 1.00 22.30 | N |
| ATOM | 93 | CA | | A1015 | 0.489 | 9.202 | 7.284 | 1.00 21.59 | C C |
| ATOM | 94 | CB | | A1015 | -0.529 | 8.372 | 8.068 | 1.00 20.65 | C |
| ATOM | 95 | C | | A1015 | 0.664 | 10.568 | 7.938 | 1.00 21.21 | 0 |
| MOTA | 96 | 0 | | A1015 | 0.101 | 11.562 | 7.483 | 1.00 19.58 | И |
| ATOM | 97 | N | | A1016 | 1.442 | 10.605 | 9.017 | 1.00 21.38 | C |
| MOTA | 98 | CA | | A1016 | 1.711 | 11.848 | 9.728 | 1.00 22.18 1.00 22.67 | c |
| MOTA | 99 | CB | | A1016 | 2.587 | 11.569 | 10.951 | 1.00 22.67 | 0 |
| ATOM | 100 | OG | | A1016 | 2.034 | 10.523 | 11.733 | 1.00 29.04 | c |
| ATOM | 101 | С | | A1016 | 2.428 | 12.825 | 8.800 | 1.00 22.03 | 0 |
| ATOM | 102 | 0 | | A1016 | 2.134 | 14.020 | 8.786 | 1.00 24.56 | N N |
| ATOM | 103 | N | | A1017 | 3.382 | 12.319 | 8.027 | 1.00 21.30 | C |
| ATOM | 104 | CA | | A1017 | 4.112 | 13.177 | 7.104 | 1.00 22.10 | C |
| ATOM | 105 | CB | | A1017 | 5.336 | 12.454 | 6.523 | 1.00 22.24 | C |
| ATOM | 106 | | | A1017 | 5.975 | 13.312 | 5.432 7.641 | 1.00 21.89 | č |
| ATOM | 107 | | | A1017 | 6.342 | 12.174 13.440 | 8.287 | 1.00 22.38 | Č |
| ATOM | 108 | | | A1017 | 6.904 3.207 | 13.440 | 5.957 | 1.00 24.27 | c |
| ATOM | 109 | C | | A1017 | 3.244 | 14.793 | 5.549 | 1.00 22.55 | Ö |
| ATOM | 110 | 0 | | A1017 A1018 | 2.388 | 12.726 | 5.440 | 1.00 23.95 | N |
| ATOM | 111 | N C7 | | A1018 | 1.494 | 13.096 | 4.348 | 1.00 26.57 | C |
| ATOM | 112 113 | CA CB | | A1018 | 0.794 | 11.862 | 3.775 | 1.00 29.38 | C |
| MOTA | 114 | CG | | A1018 | -0.244 | 12.197 | 2.709 | 1.00 33.05 | С |
| ATOM ATOM | 115 | CD | | A1018 | -0.655 | 10.987 | 1.900 | 1.00 36.21 | С |
| ATOM | 116 | | | A1018 | -0.803 | 9.897 | 2.495 | 1.00 38.49 | 0 |
| ATOM | 117 | | | A1018 | -0.840 | 11.131 | 0.672 | 1.00 38.02 | 0 |
| ATOM | 118 | C | | A1018 | 0.466 | 14.116 | 4.819 | 1.00 25.75 | С |
| ATOM | 119 | Ö | | A1018 | 0.115 | 15.032 | 4.082 | 1.00 25.64 | 0 |
| ATOM | 120 | N | | A1019 | -0.011 | 13.960 | 6.052 | 1.00 27.25 | N |
| ATOM | 121 | CA | | A1019 | -0.980 | 14.893 | 6.615 | 1.00 27.84 | C |
| ATOM | 122 | CB | | A1019 | -1.436 | 14.425 | 8.000 | 1.00 28.92 | С |
| ATOM | 123 | OG | SEF | A1019 | -2.107 | 13.176 | 7.929 | 1.00 31.15 | 0 |
| ATOM | 124 | С | SEF | A1019 | -0.338 | 16.275 | 6.734 | 1.00 28.62 | С |
| MOTA | 125 | 0 | SEF | R A1019 | -0.956 | 17.289 | 6.400 | 1.00 27.65 | 0 |
| MOTA | 126 | N | ALA | A1020 | 0.907 | 16.302 | 7.209 | 1.00 28.27 | N |
| MOTA | 127 | CA | ALF | A1020 | 1.650 | 17.545 | 7.374 | 1.00 30.56 | С |
| ATOM | 128 | CB | ALA | A1020 | 3.020 | 17.267 | 8.005 | 1.00 30.65 | C |
| ATOM | 129 | С | ALA | A1020 | 1.823 | 18.267 | 6.045 | 1.00 31.87 | C |
| ATOM | 130 | 0 | ALA | A A1020 | 1.686 | 19.487 | 5.976 | 1.00 32.82 | 0 |
| ATOM | 131 | N | | . A1021 | 2.127 | 17.513 | 4.992 | 1.00 33.76 | N |
| MOTA | 132 | CA | | A1021 | 2.304 | 18.099 | | 1.00 34.05 | С |
| ATOM | 133 | CB | | A1021 | 2.830 | 17.057 | 2.656 | | С |
| ATOM | 134 | | | L A1021 | 2.878 | 17.660 | | 1.00 31.58 | C |
| ATOM | 135 | CG2 | AV S | L A1021 | 4.213 | 16.577 | 3.073 | 1.00 33.12 | С |

| MOTA | 136 | С | VAT. | A1021 | 0.969 | 18.635 | 3.150 | 1.00 35 | .65 | С |
|------|------|------|------|---------|--------|--------|--------|---------|-------|---|
| ATOM | 137 | 0 | | A1021 | 0.891 | 19.754 | 2.643 | 1.00 34 | .17 | 0 |
| ATOM | 138 | N | | A1022 | -0.081 | 17.829 | 3.294 | 1.00 36 | .17 | N |
| ATOM | 139 | CA | | A1022 | -1.418 | 18.209 | 2.842 | 1.00 37 | .29 | С |
| | | CB | | A1022 | -2.433 | 17.074 | 3.096 | 1.00 35 | | С |
| ATOM | 140 | | | A1022 | -2.107 | 15.955 | 2.265 | 1.00 34 | | 0 |
| ATOM | 141 | | | A1022 | -3.845 | 17.530 | 2.776 | 1.00 35 | | С |
| ATOM | 142 | | | A1022 | -1.933 | 19.482 | 3.504 | 1.00 39 | | С |
| ATOM | 143 | C | | | -2.672 | 20.250 | 2.885 | 1.00 38 | | 0 |
| ATOM | 144 | 0 | | A1022 | -1.544 | 19.702 | 4.758 | 1.00 42 | | N |
| ATOM | 145 | N | | A1023 | -1.977 | 20.885 | 5.496 | 1.00 46 | | С |
| ATOM | 146 | CA | | A1023 | | 20.727 | 6.991 | 1.00 48 | | C |
| ATOM | 147 | CB | | A1023 | -1.684 | 19.534 | 7.664 | 1.00 51 | | C |
| ATOM | 148 | CG | | A1023 | -2.327 | 19.477 | 9.125 | 1.00 55 | | Ċ |
| ATOM | 149 | CD | | A1023 | -1.900 | 18.208 | 9.770 | 1.00 59 | | N |
| ATOM | 150 | NE | | A1023 | -2.234 | | 11.039 | 1.00 61 | | C |
| MOTA | 151 | CZ | | A1023 | -1.958 | 17.922 | | 1.00 61 | | N |
| MOTA | 152 | | | A1023 | 1.344 | 18.818 | 11.804 | 1.00 63 | | N |
| MOTA | 153 | NH2 | | A1023 | -2.292 | 16.741 | 11.546 | | | C |
| ATOM | 154 | С | | A1023 | -1.275 | 22.147 | 4.999 | 1.00 4 | | 0 |
| MOTA | 155 | 0 | | A1023 | -1.801 | 22.888 | 4.166 | 1.00 4 | | N |
| MOTA | 156 | N | | A1024 | -0.077 | 22.381 | 5.526 | 1.00 49 | | C |
| MOTA | 157 | CA | | A1024 | 0.714 | 23.553 | 5.171 | 1.00 49 | | C |
| ATOM | 158 | CB | HIS | A1024 | 1.238 | 24.226 | 6.441 | 1.00 5 | | C |
| ATOM | 159 | CG | HIS | A1024 | 1.367 | 23.295 | 7.608 | 1.00 5 | | |
| ATOM | 160 | CD2 | HIS | A1024 | 2.447 | 22.670 | 8.136 | 1.00 5 | | C |
| ATOM | 161 | | | A1024 | 0.284 | 22.885 | 8.357 | 1.00 5 | | N |
| MOTA | 162 | CE1 | HIS | A1024 | 0.691 | 22.048 | 9.295 | 1.00 5 | | C |
| ATOM | 163 | NE2 | HIS | A1024 | 1.999 | 21.900 | 9.183 | 1.00 5 | | N |
| ATOM | 164 | С | HIS | A1024 | 1.877 | 23.218 | 4.249 | 1.00 4 | | C |
| MOTA | 165 | 0 | HIS | A1024 | 2.655 | 22.296 | 4.513 | 1.00 4 | | 0 |
| MOTA | 166 | N | GLU | J A1025 | 1.987 | 23.983 | 3.167 | 1.00 4 | | N |
| MOTA | 167 | CA | GLU | J A1025 | 3.043 | 23.796 | 2.179 | 1.00 4 | | C |
| ATOM | 168 | CB | GLU | J A1025 | 2.813 | 24.722 | 0.984 | 1.00 5 | | C |
| MOTA | 169 | CG | GLU | J A1025 | 3.876 | 24.605 | -0.092 | 1.00 5 | | C |
| ATOM | 170 | CD | GL | J A1025 | 4.200 | 25.938 | -0.735 | 1.00 5 | | C |
| ATOM | 171 | OE1 | GL | J A1025 | 3.295 | 26.547 | -1.343 | 1.00 5 | | 0 |
| ATOM | 172 | OE2 | GL | J A1025 | 5.365 | 26.377 | -0.627 | 1.00 5 | | 0 |
| MOTA | 173 | С | GL | J A1025 | 4.418 | 24.081 | 2.768 | 1.00 4 | | С |
| ATOM | 174 | 0 | GL | J A1025 | 5.433 | 23.604 | 2.258 | 1.00 4 | | 0 |
| ATOM | 175 | N | GL' | Y A1026 | 4.447 | 24.859 | 3.845 | 1.00 4 | | N |
| ATOM | 176 | CA | GL: | Y A1026 | 5.709 | 25.202 | 4.474 | 1.00 3 | | С |
| ATOM | 177 | С | GL | Y A1026 | 6.425 | 24.069 | 5.192 | 1.00 3 | | C |
| ATOM | 178 | 0 | GL' | Y A1026 | 7.572 | 24.235 | 5.608 | 1.00 3 | | 0 |
| ATOM | 179 | N | PH | E A1027 | 5.771 | 22.920 | 5.337 | 1.00 3 | | N |
| MOTA | 180 | CA | PH | E A1027 | 6.390 | 21.791 | 6.028 | 1.00 | | С |
| ATOM | 181 | CB | PH | E A1027 | 5.397 | 20.637 | 6.179 | 1.00 | | С |
| ATOM | 182 | CG | PH | E A1027 | 5.951 | 19.469 | 6.951 | 1.00 3 | 30.68 | С |
| ATOM | 183 | | 1 PH | E A1027 | 6.224 | 19.586 | 8.312 | 1.00 2 | | С |
| MOTA | 184 | | | E A1027 | 6.230 | 18.266 | 6.313 | 1.00 | | С |
| ATOM | 185 | | | E A1027 | 6.768 | 18.523 | 9.027 | 1.00 | | С |
| ATOM | 186 | | | E A1027 | 6.775 | | 7.020 | 1.00 | | С |
| MOTA | 187 | | | E A1027 | 7.045 | | 8.383 | 1.00 | | С |
| MOTA | 188 | | | E A1027 | 7.653 | | 5.345 | 1.00 | 29.93 | С |
| ATOM | 189 | | | E A1027 | 8.741 | | 5.908 | 1.00 | | 0 |
| ATOM | 190 | | | A A1028 | 7.504 | | | 1.00 | | N |
| ATOM | 191 | | | A A1028 | 8.637 | | | | 28.78 | С |
| ATOM | 192 | | | A A1028 | 8.213 | | | | 28.60 | C |
| ALON | 1 72 | . 01 | | | | | | | | |

| ATOM | 193 | С | ALA | A1028 | 9.779 | 21.204 | 3.371 | 1.00 29.38 | С |
|--------------|------------|--------|-----|----------------|------------------|---------------|------------------|--------------------------|--------|
| MOTA | 194 | 0 | ALA | A1028 | 10.940 | 20.850 | 3.579 | 1.00 28.07 | 0 |
| MOTA | 195 | N | | A1029 | 9.424 | 22.463 | 3.127 | 1.00 30.57 | N |
| ATOM | 196 | CA | LYS | A1029 | 10.372 | 23.574 | 3.062 | 1.00 32.15 | С |
| ATOM | 197 | СВ | | A1029 | 9.608 | 24.867 | 2.765 | 1.00 34.73 | С |
| ATOM | 198 | CG | | A1029 | 10.076 | 25.630 | 1.535 | 1.00 38.51 | С |
| ATOM | 199 | CD | | A1029 | 11.365 | 26.404 | 1.799 | 1.00 41.30 | С |
| MOTA | 200 | CE | | A1029 | 11.653 | 27.390 | 0.669 | 1.00 41.77 | C |
| ATOM | 201 | NZ | | A1029 | 12.865 | 28.214 | 0.927 | 1.00 43.68 | N |
| ATOM | 202 | С | | A1029 | 11.173 | 23.729 | 4.357 | 1.00 31.51 | C |
| ATOM | 203 | 0 | | A1029 | 12.362 | 24.043 | 4.326 | 1.00 31.47 | 0 |
| ATOM | 204 | N | | A1030 | 10.521 | 23.512 | 5.495 | 1.00 31.52 | N |
| ATOM | 205 | CA | | A1030 | 11.195 | 23.626 | 6.787 | 1.00 32.17 | С |
| ATOM | 206 | СВ | ARG | A1030 | 10.188 | 23.625 | 7.949 | 1.00 34.49 | С |
| ATOM | 207 | CG | | A1030 | 9.287 | 24.838 | | 1.00 38.44 | С |
| ATOM | 208 | CD | | A1030 | 8.775 | 25.030 | 9.497 | 1.00 41.54 | С |
| ATOM | 209 | NE | | A1030 | 8.304 | 23.796 | 10.134 | 1.00 44.99 | N |
| ATOM | 210 | CZ | | A1030 | 9.084 | 22.932 | 10.786 | 1.00 47.20 | C |
| ATOM | 211 | | | A1030 | 10.388 | 23.157 | 10.898 | 1.00 48.13 | N |
| MOTA | 212 | | | A1030 | .8.562 | 21.841 | 11.337 | 1.00 47,12 | N |
| ATOM | 213 | С | | A1030 | 12.145 | 22.460 | 7.013 | 1.00 30.09 | С |
| ATOM | 214 | 0 | ARG | A1030 | 13.248 | 22.631 | 7.530 | 1.00 29.93 | 0 |
| MOTA | 215 | N | VAL | A1031 | 11.696 | 21.272 | 6.628 | 1.00 27.81 | N |
| MOTA | 216 | CA | | A1031 | 12.460 | 20.050 | 6.819 | 1.00 25.50 | С |
| ATOM | 217 | CB | VAL | A1031 | 11.531 | 18.806 | 6.723 | 1.00 24.73 | С |
| ATOM | 218 | CG1 | VAL | A1031 | 12.355 | 17.518 | 6.871 | 1.00 24.35 | C |
| ATOM | 219 | CG2 | VAL | A1031 | 10.465 | 18.874 | 7.798 | 1.00 23.33 | С |
| ATOM | 220 | С | VAL | A1031 | 13.621 | 19.835 | 5.861 | 1.00 25.01 | С |
| ATOM | 221 | 0 | VAL | A1031 | 14.664 | 19.307 | 6.252 | 1.00 25.89 | 0 |
| ATOM | 222 | N | LEU | A1032 | 13.451 | 20.253 | 4.617 | 1.00 24.38 | N |
| MOTA | 223 | CA | LEU | A1032 | 14.472 | 20.027 | 3.604 | 1.00 25.25 | С |
| MOTA | 224 | CB | LEU | A1032 | 13.818 | 19.409 | 2.370 | 1.00 25.23 | С |
| MOTA | 225 | CG | LEU | A1032 | 12.870 | 18.230 | 2.597 | 1.00 23.47 | С |
| MOTA | 226 | | | A1032 | 12.275 | 17.806 | 1.266 | 1.00 23.54 | С |
| ATOM | 227 | CD2 | | A1032 | 13.624 | 17.072 | 3.239 | 1.00 23.54 | С |
| MOTA | 228 | С | LEU | A1032 | 15.271 | 21.243 | 3.169 | 1.00 25.67 | С |
| MOTA | 229 | 0 | | A1032 | 14.778 | 22.371 | 3.184 | 1.00 25.62 | 0 |
| ATOM | 230 | N | | A1033 | 16.516 | 20.997 | 2.776 | 1.00 26.32 | N |
| ATOM | 231 | CA | | A1033 | 17.387 | 22.057 | 2.289 | 1.00 27.40 | C |
| ATOM | 232 | CB | | A1033 | 18.862 | 21.628 | 2.283 | 1.00 27.76 | С |
| ATOM | 233 | | | A1033 | 19.015 | 20.490 | 1.425 | 1.00 26.35 | 0 |
| ATOM | 234 | | | A1033 | 19.331 | 21.271 | 3.691 | 1.00 28.10 | C |
| MOTA | 235 | C | | A1033 | .16.963 | 22.275 | 0.844 | 1.00 27.65 | C |
| ATOM | 236 | 0 | | A1033 | 16.071 | 21.588 | 0.350 | 1.00 27.78 | 0 |
| ATOM | 237 | N | | A1034 | 17.612 | 23.215 | 0.166 | 1.00 27.93 | N |
| ATOM | 238 | | | A1034 | | | | 1.00 28.06 | C |
| ATOM | 239 | CB | | A1034 A1034 | 18.089 | 24.717 22.296 | -1.695 -2.119 | 1.00 29.35 | C |
| ATOM ATOM | 240 241 | С 0 | | | 17.594 | 22.296 | | 1.00 27.67 | С |
| ATOM | 242 | N | | A1034 A1035 | 16.791 18.752 | 21.675 | -2.981 -1.918 | 1.00 28.26 1.00 27.21 | О И |
| ATOM | 243 | CA | | A1035 | 19.131 | 20.510 | -2.711 | 1.00 27.21 | C |
| ATOM | 244 | CB | | A1035 | 20.531 | 20.510 | -2.711 | 1.00 29.21 | C |
| ATOM | 245 | CG | | A1035 | 21.743 | 20.903 | -2.634 | 1.00 28.30 | C |
| ATOM | 246 | | | A1035 | 22.960 | 20.382 | -1.877 | 1.00 32.40 | č |
| ATOM | 247 | | | A1035 | 22.017 | 20.924 | -4.137 | 1.00 32.53 | Ċ |
| ATOM | 248 | C | | A1035 | 18.111 | 19.388 | -2.514 | 1.00 27.97 | Ċ |
| ATOM | 249 | ŏ | | A1035 | 17.674 | 18.758 | -3.475 | 1.00 28.70 | o |
| | | | | | - | _ | _ | • • | |

| | | | | | | | | | | 7 07 | NT. |
|--------------|------------|-----|-----|--------------------|---|----------|--------|--------------------|--------|-------|--------|
| MOTA | 250 | N | GLU | A1036 | • | 17.731 | | -1.267 | 1.00 2 | | N |
| ATOM | 251 | CA | - | A1036 | | 16.757 | 18.100 | -0.980 | 1.00 2 | | C C |
| ATOM | 252 | CB | | A1036 | | 16.599 | 17.938 | 0.532 | 1.00 2 | | C |
| ATOM | 253 | CG | GLU | A1036 | | 17.760 · | 17.195 | 1.186 | 1.00 2 | | |
| MOTA | 254 | CD | | A1036 | | 17.720 | 17.252 | 2.703 | 1.00 2 | | С |
| ATOM | 255 | OE1 | GLU | A1036 | | 18.225 | 16.306 | 3.345 | 1.00 2 | | 0 |
| ATOM | 256 | OE2 | GLU | A1036 | | 17.201 | 18.248 | 3.256 | 1.00 2 | | 0 |
| ATOM | 257 | С | GLU | A1036 | | 15.413 | 18.416 | -1.634 | 1.00 2 | | C |
| ATOM | 258 | 0 | GLU | A1036 | | 14.740 | 17.522 | -2.138 | 1.00 2 | | 0 |
| ATOM | 259 | N | MET | A1037 | | 15.031 | 19.691 | -1.640 | 1.00 2 | | N |
| ATOM | 260 | CA | MET | A1037 | | 13.765 | 20.099 | -2.247 | 1.00 2 | | С |
| ATOM | 261 | СВ | MET | A1037 | | 13.529 | 21.599 | -2.06 9 | 1.00 3 | | С |
| ATOM | 262 | CG | MET | A1037 | | 12.985 | 22.000 | -0.714 | 1.00 3 | | С |
| ATOM | 263 | SD | MET | A1037 | | 11.412 | 21.198 | -0.336 | 1.00 3 | | S |
| ATOM | 264 | CE | | Á1037 | | 10.356 | 21.852 | -1.624 | 1.00 3 | 3.04 | С |
| ATOM | 265 | C | | A1037 | | 13.758 | 19.779 | -3.731 | 1.00 3 | | С |
| ATOM | 266 | Ō | | A1037 | | 12.711 | 19.461 | -4.306 | 1.00 3 | | 0 |
| ATOM | 267 | N | | A1038 | | 14.928 | 19.881 | -4.352 | 1.00 3 | 31.50 | N |
| ATOM | 268 | CA | | A1038 | | 15.049 | 19.600 | -5.774 | 1.00 3 | 33.14 | C |
| ATOM | 269 | CB | | A1038 | | 16.499 | 19.777 | -6.233 | 1.00 3 | 34.77 | С |
| ATOM | 270 | CG | | A1038 | | 17.005 | 21.208 | -6.093 | 1.00 3 | 39.68 | С |
| ATOM | 271 | CD | | A1038 | | 18.411 | 21.400 | -6.639 | 1.00 4 | 11.20 | С |
| ATOM | 272 | | | A1038 | | 18.981 | 22.492 | -6.434 | 1.00 4 | 14.15 | 0 |
| ATOM | 273 | | | A1038 | | 18.943 | 20.467 | -7.276 | 1.00 4 | 12.51 | 0 |
| ATOM | 274 | C | | A1038 | | 14.570 | 18.186 | -6.066 | 1.00 | 31.14 | C |
| ATOM | 275 | o | | A1038 | | 13.773 | 17.974 | -6.976 | 1.00 | | 0 |
| ATOM | 276 | N | | A1039 | | 15.039 | 17.215 | -5.290 | 1.00 | | N |
| | 277 | CA | | A1039 | | 14.606 | 15.844 | -5.521 | 1.00 | | C |
| ATOM | 278 | CB | | A1039 | | 15.499 | 14.846 | -4.778 | 1.00 | 29.96 | C |
| ATOM | 279 | CG | | A1039 | | 15.061 | 13.406 | -5.005 | 1.00 | | С |
| ATOM | 280 | CD | | A1039 | | 16.213 | 12.420 | -4.969 | 1.00 | | С |
| ATOM | 281 | NE | | A1039 | | 15.723 | 11.046 | -5.085 | 1.00 | | N |
| MOTA | | CZ | | A1039 | | 15.203 | 10.509 | -6.188 | 1.00 | | С |
| MOTA | 282 283 | | | A1039 | | 15.098 | 11.214 | -7.310 | 1.00 | | N |
| ATOM | 284 | | | A1039 | | 14.764 | 9.258 | -6.161 | 1.00 | | N |
| ATOM | 285 | C | | A1039 | | 13.158 | 15.671 | -5.086 | 1.00 | | C |
| ATOM | 286 | 0 | | A1039 | | 12.367 | 15.046 | -5.785 | 1.00 | | 0 |
| ATOM ATOM | 287 | Ŋ | | A1040 | | 12.808 | 16.233 | -3.934 | | 24.86 | N |
| ATOM | 288 | CA | | A1040 | | 11.441 | 16.132 | -3.430 | | 26.03 | С |
| ATOM | 289 | СВ | | E A1040 | | 11.273 | 17.007 | -2.178 | 1.00 | 25.44 | С |
| ATOM | 290 | CG | | E A1040 | | 9.861 | 17.056 | -1.657 | | 26.41 | C |
| ATOM | 291 | | | E A1040 | | 9.298 | | -1.027 | 1.00 | 25.83 | C |
| ATOM | 292 | | | E A1040 | | 9.080 | 18.194 | -1.838 | | 26.12 | С |
| ATOM | 293 | | | E A1040 | | 7.977 | 15.977 | -0.585 | | 24.52 | С |
| ATOM | 294 | | | E A1040 | | | 18.232 | -1.399 | | 26.23 | C |
| | 295 | CZ | | E A1040 | | 7.202 | 17.119 | -0.772 | 1.00 | 23.77 | С |
| ATOM | 296 | C | | E A1040 | | 10.412 | 16.548 | -4.488 | 1.00 | 26.70 | С |
| MOTA | 297 | Ö | | E A1040 | | 9.438 | 15.837 | -4.731 | | 29.10 | 0 |
| ATOM ATOM | 298 | N | | R A1041 | | 10.635 | 17.691 | -5.126 | | 28.25 | N |
| | 299 | | | R A1041 | | 9.705 | | -6.136 | | 30.17 | С |
| ATOM | 300 | CB | | R A1041 | | 9.935 | 19.700 | -6.391 | | 31.11 | C |
| ATOM | 301 | | | R A1041 | | 11.255 | | -6.904 | | 32.37 | 0 |
| MOTA | 301 | | | R A1041 | | 9.781 | | | | 29.66 | С |
| MOTA | 302 | | | R A1041 | | 9.751 | | | | 31.98 | C |
| ATOM | | | | R A1041 | | 8.863 | | | | 32.84 | 0 |
| ATOM | 304 305 | | | R A1041 R A1042 | | 10.781 | | | | 31.91 | . N |
| ATOM | 305 | | | R A1042 R A1042 | | 10.933 | | | | 32.77 | C |
| ATOM | 300 | CA | 35 | I HIU42 | | 10.755 | 13.002 | | | | |

| ATOM | 307 | CB | SER | A1042 | 12.416 | 15.609 | -9.192 | 1.00 3 | 3.18 | | С |
|------|-----|----------|-----|-------|--------|--------|---------|--------|------|----------|---|
| ATOM | 308 | OG | | A1042 | 13.106 | 16.820 | -9.448 | 1.00 3 | | | 0 |
| MOTA | 309 | C | | A1042 | 10.215 | 14.529 | -8.831 | 1.00 3 | | | C |
| ATOM | 310 | 0 | | A1042 | 10.071 | 13.834 | -9.840 | 1.00 3 | | | 0 |
| ATOM | 311 | N | | A1043 | 9.766 | 14.175 | -7.630 | 1.00 2 | | | N |
| ATOM | 312 | CA | | A1043 | 9.101 | 12.901 | -7.394 | 1.00 2 | | | Ċ |
| ATOM | 313 | CB | | A1043 | 9.541 | 12.332 | -6.043 | 1.00 2 | | | Č |
| ATOM | 314 | CG | | A1043 | 11.050 | 12.097 | -5.928 | 1.00 2 | | | č |
| ATOM | 315 | | | A1043 | 11.391 | 11.610 | -4.538 | 1.00 1 | | | č |
| ATOM | 316 | | | A1043 | 11.493 | 11.073 | -6.977 | 1.00 2 | | | Č |
| ATOM | 317 | C | | A1043 | 7.587 | 12.967 | -7.454 | 1.00 3 | | | č |
| ATOM | 318 | Ō | | A1043 | 6.995 | 14.045 | -7.415 | 1.00 2 | | | Ö |
| ATOM | 319 | N | | A1044 | 6.970 | 11.793 | -7.524 | 1.00 3 | | | N |
| ATOM | 320 | CA | | A1044 | 5.525 | 11.679 | | 1.00 3 | | | C |
| ATOM | 321 | CB | | A1044 | 5.167 | 11.102 | -9.008 | 1.00 3 | | | Č |
| ATOM | 322 | CG | | A1044 | 5.598 | | -10.199 | 1.00 4 | | | C |
| ATOM | 323 | CD | | A1044 | 4.583 | | -10.500 | 1.00 4 | | | Ċ |
| ATOM | 324 | CE | | A1044 | 4.793 | | -11.897 | 1.00 4 | | | č |
| ATOM | 325 | NZ | | A1044 | 3.591 | | -12.387 | 1.00 4 | | | N |
| ATOM | 326 | C | | A1044 | 4.883 | 10.801 | -6.564 | 1.00 3 | | | C |
| ATOM | 327 | 0 | | A1044 | 5.512 | 9.894 | -6.017 | 1.00 3 | | | Ö |
| ATOM | 328 | N | | A1044 | 3.611 | 11.080 | -6.299 | 1.00 3 | | | N |
| ATOM | 329 | CA | | A1045 | 2.834 | 10.321 | -5.337 | 1.00 3 | | | C |
| ATOM | 330 | C | | A1045 | 3.518 | 9.841 | -4.074 | 1.00 3 | | | Ċ |
| ATOM | 331 | 0 | | A1045 | 4.098 | 10.631 | -3.329 | 1.00 3 | | | 0 |
| ATOM | 332 | N | | A1045 | 3.435 | 8.534 | -3.841 | 1.00 3 | | | Ŋ |
| ATOM | 333 | | | A1046 | 4.009 | 7.904 | -2.659 | 1.00 3 | | | C |
| ATOM | 334 | CA CB | | A1046 | 3.791 | 6.386 | -2.717 | 1.00 3 | | | C |
| ATOM | 335 | CG | | A1046 | 2.420 | 5.971 | -3.239 | 1.00 4 | | | C |
| ATOM | 336 | CD | | A1046 | 2.301 | 4.457 | -3.386 | 1.00 4 | | , | C |
| ATOM | 337 | NE | | A1046 | 1.885 | 3.810 | -2.144 | 1.00 5 | | | N |
| ATOM | 338 | CZ | | A1046 | 1.793 | 2.493 | -1.980 | 1.00 5 | | | C |
| MOTA | 339 | | | A1046 | 1.399 | 1.995 | -0.815 | 1.00 5 | | | N |
| MOTA | 340 | | | A1046 | 2.106 | 1.673 | -2.975 | 1.00 5 | | | N |
| ATOM | 341 | C | | A1046 | 5.499 | 8.194 | -2.516 | 1.00 3 | | | C |
| ATOM | 342 | 0 | | A1046 | 5.972 | 8.529 | -1.433 | 1.00 3 | | | Ö |
| ATOM | 343 | N | | A1047 | 6.234 | 8.060 | -3.614 | 1.00 3 | | | N |
| MOTA | 344 | CA | | A1047 | 7.670 | 8.292 | -3.605 | 1.00 3 | | | C |
| ATOM | 345 | CB | | A1047 | 8.235 | 8.126 | -5.015 | 1.00 3 | | | C |
| ATOM | 346 | CG | | A1047 | 9.252 | 7.013 | -5.123 | 1.00 3 | | | č |
| ATOM | 347 | CD | | A1047 | 8.909 | 6.055 | -6.246 | 1.00 4 | | | č |
| ATOM | 348 | NE | | A1047 | 9.734 | 4.854 | -6.183 | 1.00 4 | | | N |
| ATOM | 349 | CZ | | A1047 | 9.635 | 3.835 | | 1.00 4 | | | C |
| ATOM | 350 | | | A1047 | 10.428 | 2.780 | | 1.00 4 | | | N |
| ATOM | 351 | | | A1047 | 8.743 | 3.873 | | 1.00 4 | | | N |
| ATOM | | С | | A1047 | 8.040 | | -3.062 | | | | C |
| ATOM | 353 | ō | | A1047 | 9.006 | -9.808 | -2.307 | 1.00 2 | | | 0 |
| ATOM | 354 | N | | A1048 | 7.268 | 10:680 | | 1.00 2 | | | N |
| ATOM | 355 | CA | | A1048 | 7.522 | 12.042 | | 1.00 2 | | | С |
| ATOM | 356 | СВ | | A1048 | 6.552 | 13.014 | -3.679 | 1.00 2 | | | С |
| ATOM | 357 | CG | | A1048 | 6.972 | 14.472 | | 1.00 2 | | | Č |
| ATOM | 358 | CD | | A1048 | 6.169 | 15.400 | | 1.00 2 | | | Č |
| ATOM | 359 | | | A1048 | 6.618 | 16.495 | | 1.00 2 | | | 0 |
| ATOM | 360 | | | A1048 | 4.977 | 14.970 | | 1.00 2 | | | N |
| ATOM | 361 | С | | A1048 | 7.390 | 12.162 | | 1.00 2 | | | С |
| ATOM | 362 | 0 | | A1048 | 8.225 | 12.783 | | 1.00 2 | | | 0 |
| ATOM | 363 | N | | A1049 | 6.340 | 11.568 | | 1.00 2 | | | N |
| | | | | | | | | | | | |

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|------|-----|-----|-----|----------|---|--------|----------|--------|------|---------|---|
| MOTA | 364 | CA | ILE | A1049 | | | 11.615 | 0.523 | | 23.77 | C |
| ATOM | 365 | CB | ILE | A1049 | | 1.733 | 11.084 | 0.900 | | 25.38 | C |
| ATOM | 366 | | | A1049 | | | 11.001 | 2.401 | | 25.87 | C |
| ATOM | 367 | CG1 | ILE | A1049 | 3 | 3.657 | 11.999 | 0.315 | | 26.78 | C |
| ATOM | 368 | CD1 | ILE | A1049 | 3 | 3.787 | 13.453 | 0.751 | | 30.33 | C |
| ATOM | 369 | С | ILE | A1049 | - | 7.181 | 10.776 | 1.228 | | 22.10 | C |
| ATOM | 370 | 0 | ILE | A1049 | - | 7.673 | 11.150 | 2.283 | | 21.61 | 0 |
| ATOM | 371 | N | GLU | A1050 | | 7.525 | 9.642 | 0.631 | | 22.60 | N |
| ATOM | 372 | CA | | A1050 | { | 8.532 | 8.755 | 1.200 | | 23.30 | С |
| ATOM | 373 | СВ | | A1050 | 8 | 8.667 | 7.478 | 0.363 | | 23.16 | С |
| ATOM | 374 | CG | | A1050 | 9 | 9.889 | 6.659 | 0.739 | | 28.58 | С |
| ATOM | 375 | CD | | A1050 | 1 | 9.978 | 6.445 | 2.234 | | 29.28 | С |
| ATOM | 376 | | | A1050 | 1 | 1.108 | 6.330 | 2.760 | | 30.35 | 0 |
| ATOM | 377 | | | A1050 | | 8.909 | 6.394 | 2.882 | 1.00 | 30.91 | 0 |
| ATOM | 378 | C | | A1050 | | 9.885 | 9.454 | 1.279 | | 22.26 | С |
| | 379 | 0 | | A1050 | | 0.627 | 9.288 | 2.253 | 1.00 | 23.12 | 0 |
| ATOM | | N | | A1051 | | 0.209 | 10.245 | 0.262 | 1.00 | 22.07 | N |
| ATOM | 380 | | | | | 1.478 | 10.948 | 0.262 | | 21.63 | С |
| ATOM | 381 | CA | | A1051 | | 1.686 | 11.704 | -1.054 | | 20.34 | С |
| ATOM | 382 | CB | | A1051 | | 2.992 | 12.472 | -1.082 | | 20.50 | С |
| ATOM | 383 | CG | | A1051 | | | 13.801 | -0.659 | | 20.43 | C |
| ATOM | 384 | | | A1051 | | 3.055 | 14.490 | -0.621 | | 20.01 | Ċ |
| MOTA | 385 | | | A1051 | | 4.269 | | -1.475 | | 20.86 | C |
| ATOM | 386 | | | A1051 | | 4.179 | 11.849 | | | 21.25 | c |
| MOTA | 387 | | | A1051 | | 5.400 | 12.531 | -1.441 | | 19.89 | C |
| ATOM | 388 | CZ | | A1051 | | 5.432 | 13.852 | -1.010 | | | Ö |
| ATOM | 389 | ОН | | A1051 | | 6.630 | 14.525 | -0.959 | | 20.04 | C |
| ATOM | 390 | С | | A1051 | | 1.557 | 11.920 | 1.434 | | 21.88 | Ö |
| ATOM | 391 | 0 | | A1051 | | 2.557 | 11.963 | 2.152 | | 20.59 | N |
| MOTA | 392 | N | LEU | A1052 | | 10.499 | 12.702 | 1.621 | | 21.63 | C |
| MOTA | 393 | CA | LEU | A1052 | 1 | 10.452 | 13.671 | 2.706 | | 21.68 | |
| MOTA | 394 | CB | LEU | 1 A1052 | | 9.179 | 14.513 | 2.590 | | 20.47 | C |
| ATOM | 395 | CG | | A1052 | | 8.808 | 15.418 | 3.765 | | 22.03 | C |
| ATOM | 396 | CD1 | LEU | J A1052 | | 9.962 | 16.348 | 4.120 | | 21.80 | С |
| ATOM | 397 | CD2 | LEU | J A1052 | | 7.566 | 16.209 | 3.381 | | 20.67 | C |
| MOTA | 398 | С | LEU | J A1052 | 1 | 10.504 | 12.964 | 4.055 | | 20.98 | С |
| ATOM | 399 | 0 | LEU | J A1052 | 1 | 11.314 | 13.306 | 4.919 | | 21.63 | 0 |
| ATOM | 400 | N | ALA | A A1053 | | 9.639 | 11.971 | 4.223 | | 19.65 | N |
| ATOM | 401 | CA | AL | A A1053 | | 9.578 | 11.190 | 5.457 | | 18.20 | C |
| MOTA | 402 | СВ | | A A1053 | | 8.567 | 10.054 | 5.299 | 1.00 | 18.13 | C |
| ATOM | 403 | С | AL | A A1053 | | 10.952 | 10.614 | 5.818 | 1.00 | 17.32 | С |
| ATOM | 404 | ō | | A A1053 | | 11.356 | 10.642 | 6.982 | 1.00 | 15.65 | 0 |
| ATOM | 405 | N | GL' | Y A1054 | | 11.660 | 10.092 | 4.816 | 1.00 | 16.84 | N |
| ATOM | 406 | | | Y A1054 | | 12.978 | 9.516 | 5.049 | | 16.81 | С |
| ATOM | 407 | | | Y A1054 | | 13.981 | 10.540 | 5.542 | 1.00 | 16.80 | С |
| ATOM | 408 | | | Y A1054 | | | 10.270 | 6.439 | 1.00 | 16.69 | 0 |
| ATOM | 409 | | | G A1055 | | 13.946 | 11.728 | 4.952 | 1.00 | 18.02 | N |
| ATOM | 410 | | | G A1055 | | 14.866 | | 5.364 | 1.00 | 18.20 | С |
| ATOM | 411 | | | G A1055 | | 14.811 | | 4.371 | | 19.98 | С |
| | | | | G A1055 | | 15.908 | | .3.303 | | 0 19.89 | С |
| MOTA | 412 | | | G A1055 | | 15.963 | | 2.565 | | 0 21.10 | С |
| MOTA | 413 | | | G A1055 | | 17.109 | | | | 0 21.61 | N |
| MOTA | 414 | | | G A1055 | | 17.449 | | | | 0 21.69 | С |
| MOTA | 415 | | | G A1055 | | 16.730 | | | | 0 20.97 | N |
| ATOM | 416 | | | | | 18.508 | | | | 0 17.88 | N |
| ATOM | 417 | | | G A1055 | | 14.534 | | | | 0 18.74 | C |
| ATOM | 418 | | | G A1055 | | 15.433 | | | | 0 16.13 | 0 |
| ATOM | 419 | | | G A1055 | | 13.243 | | | | 0 17.18 | N |
| ATOM | 420 |) N | TH | RP A1056 | | 10.443 | , 10.029 | | | | |

| | | | | | | | | • | | |
|--------------|------------|----------------|-----|----------------|------------------|------------------|------------------|--------------------------|---|-----|
| ATOM | 421 | CA | TRP | A1056 | 12.793 | 13.732 | 8.412 | 1.00 19.43 | | С |
| ATOM | 422 | CB | TRP | A1056 | 11.267 | 13.703 | 8.468 | 1.00 21.99 | | С |
| ATOM | 423 | CG | TRP | A1056 | 10.694 | 14.264 | 9.713 | 1.00 26.53 | | С |
| ATOM | 424 | | | A1056 | 10.311 | 13.533 | 10.877 | 1.00 28.20 | | С |
| ATOM | 425 | CE2 | TRP | A1056 | 9.816 | 14.468 | 11.813 | 1.00 28.53 | | С |
| ATOM | 426 | CE3 | TRP | A1056 | 10.333 | 12.177 | 11.222 | 1.00 29.04 | | С |
| ATOM | 427 | CD1 | TRP | A1056 | 10.431 | 15.581 | 9.978 | 1.00 26.38 | | С |
| MOTA | 428 | NE1 | TRP | A1056 | 9.905 | 15.708 | 11.237 | 1.00 29.97 | | N |
| ATOM | 429 | CZ2 | TRP | A1056 | 9.347 | 14.090 | 13.073 | 1.00 30.15 | | С |
| ATOM | 430 | CZ3 | TRP | A1056 | 9.868 | .11.801 | 12.476 | 1.00 31.30 | | С |
| ATOM | 431 | CH2 | TRP | A1056 | 9.379 | 12.755 | 13.386 | 1.00 31.45 | | С |
| MOTA | 432 | С | TRP | A1056 | 13.343 | 12.710 | 9.412 | 1.00 18.72 | | С |
| ATOM | 433 | 0 | TRP | A1056 | 13.992 | 13.063 | 10.397 | 1.00 16.51 | | 0 |
| ATOM | 434 | N | SER | A1057 | 13.084 | 11.435. | 9.137 | 1.00 17.50 | | N |
| ATOM | 435 | CA | SER | A1057 | 13.532 | 10.352 | 10.011 | 1.00 19.23 | | С |
| MOTA | 436 | CB | SER | A1057 | 13.053 | 9.009 | 9.448 | 1.00 21.41 | | С |
| MOTA | 437 | OG | SER | A1057 | 13.243 | 7.971 | 10.388 | 1.00 25.06 | | 0 |
| ATOM | 438 | С | SER | A1057 | 15.053 | 10.320 | 10.201 | 1.00 19.01 | | С |
| MOTA | 439 | 0 | SER | A1057 | 15.549 | 10.120 | 11.317 | 1.00 19.71 | | 0 |
| MOTA | 440 | N | ALA | A1058 | 15.789 | 10.511 | 9.111 | 1.00 16.54 | | N |
| MOTA | 441 | CA | ALA | A1058 | 17.243 | 10.495 | 9.162 | 1.00,16.02 | | С |
| ATOM | 442 | CB | ALA | A1058 | 17.798 | 10.607 | 7.757 | 1.00 15.16 | | С |
| ATOM | 443 | С | | A1058 | 17.790 | 11.616 | 10.035 | 1.00 15.70 | | С |
| ATOM | 444 | 0 | | A1058 | 18.707 | 11.411 | 10.836 | 1.00 16.78 | | 0 |
| MOTA | 445 | N | LYS | A1059 | 17.221 | 12.805 | 9.884 | 1.00 16.69 | | N |
| MOTA | 446 | CA | | A1059 | 17.664 | 13.957 | 10.648 | 1.00 18.17 | | C |
| ATOM | 447 | CB | | A1059 | 17.079 | 15.240 | 10.042 | 1.00 18.92 | | С |
| MOTA | 448 | CG | | A1059 | 17.536 | 15.450 | 8.588 | 1.00 19.75 | | С |
| ATOM | 449 | CD | | A1059 | 17.059 | 16.773 | 8.003 | 1.00 19.99 | | С |
| ATOM | 450 | CE | | A1059 | 17.531 | 16.933 | 6.549 | 1.00 19.86 | | С |
| ATOM | 451 | NZ | | A1059 | 17.304 | 18.322 | 6.031 | 1.00 20.25 | | N |
| ATOM | 452 | С | | A1059 | 17.302 | 13.818 | 12.116 | 1.00 19.11 | | С |
| ATOM | 453 | 0 | | A1059 | 18.067 | 14.222 | 12.995 | 1.00 18.56 | | 0 |
| ATOM | 454 | N | | A1060 | 16.143 | 13.225 | 12.374 | 1.00 18.52 | | N |
| ATOM | 455 | CA | | A1060 | 15.679 | 12.998 | 13.736 | 1.00 21.84 | | C |
| ATOM | 456 | CB | | A1060 | 14.247 | 12.448 | 13.704 | 1.00 26.26 | | С |
| MOTA | 457 458 | CG CD | | A1060 A1060 | 13.428 13.083 | 12.722 14.192 | 14.952 15.130 | 1.00 33.87 1.00 35.47 | | C |
| MOTA | 459 | | | A1060 | 12.298 | 14.192 | 14.322 | 1.00 33.47 | | 0 |
| ATOM ATOM | 460 | | | A1060 | 13.601 | 14.733 | 16.082 | 1.00 38.74 | | 0 |
| MOTA | 461 | C | | A1060 | 16.631 | 11.982 | 14.390 | 1.00 21.03 | | C |
| ATOM | 462 | 0 | | A1060 | 17.045 | 12.149 | 15.544 | 1.00 21.03 | | 0 |
| ATOM | 463 | N | | A1061 | 16.991 | 10.943 | 13.635 | 1.00 18.55 | | N |
| ATOM | 464 | CA | | A1061 | 17.898 | 9.910 | 14.131 | 1.00 18.39 | | C |
| ATOM | 465 | CB | | A1061 | 18.017 | | 13.113 | | | c ´ |
| ATOM | 466 | C | | A1061 | 19.283 | 10.490 | 14.429 | 1.00 18.00 | | C |
| ATOM | 467 | ō | | A1061 | | 10.151 | 15.436 | 1.00 17.16 | | 0 |
| ATOM | 468 | N | | A1062 | 19.768 | 11.352 | 13.542 | 1.00 18.20 | • | N |
| ATOM | 469 | CA | | A1062 | 21.069 | 11.970 | 13.741 | 1.00 20.25 | | C |
| ATOM | 470 | СВ | | A1062 | 21.433 | 12.855 | 12.546 | 1.00 20.89 | | С |
| MOTA | 471 | CG | | A1062 | 22.721 | 13.605 | 12.730 | 1.00 23.32 | | С |
| ATOM | 472 | | | A1062 | 22.761 | 14.776 | 13.489 | 1.00 24.72 | | С |
| ATOM | 473 | CD2 | PHE | A1062 | 23.908 | 13.112 | 12.194 | 1.00 23.55 | | С |
| MOTA | 474 | CE1 | PHE | A1062 | 23.973 | 15.443 | . 13.717 | 1.00 24.71 | | С |
| ATOM | 475 | CE2 | PHE | A1062 | 25.119 | | 12.414 | 1.00 23.92 | | С |
| MOTA | 476 | CZ | PHE | A1062 | 25.150 | 14.934 | 13.179 | 1.00 25.42 | | С |
| MOTA | 477 | c ['] | PHE | A1062 | 21.090 | 12.800 | 15.026 | 1.00 21.33 | | С |
| | | | | | | | | | | |

| ATOM | 478 | 0 | PHE | A1062 | 22.035 | 12.726 | 15.809 | 1.00 20.18 | 0 |
|--------------|------------|--------|--------|----------------|------------------|------------------|------------------|--------------------------|--------|
| MOTA | 479 | N | SER | A1063 | 20.045 | 13.593 | 15.244 | 1.00 22.52 | N |
| ATOM | 480 | CA | SER | A1063 | 19.973 | 14.420 | 16.445 | 1.00 24.40 | C |
| ATOM | 481 | CB | SER | A1063 | 18.679 | 15.230 | 16.447 | 1.00 25.96 | С |
| ATOM | 482 | OG | SER | A1063 | 18.670 | 16.112 | 15.338 | 1.00 30.50 | 0 |
| ATOM | 483 | С | SER | A1063 | 20.060 | 13.562 | 17.704 | 1.00 24.30 | С |
| ATOM | 484 | 0 | SER | A1063 | 20.714 | 13.938 | 18.682 | 1.00 23.77 | 0 |
| ATOM | 485 | N | | A1064 | 19.407 | 12.406 | 17.678 | 1.00 22.33 | N |
| ATOM | 486 | CA | | A1064 | 19.451 | 11.513 | 18.823 | 1.00 23.04 | С |
| ATOM | 487 | СВ | | A1064 | 18.405 | 10.406 | 18.684 | 1.00 23.38 | С |
| ATOM | 488 | CG | | A1064 | 16.971 | 10.881 | 18.903 | 1.00 25.10 | Ċ |
| ATOM | 489 | CD | | A1064 | 15.986 | 9.734 | 18.726 | 1.00 28.41 | Ċ |
| ATOM | 490 | CE | | A1064 | 14.548 | 10.194 | 18.924 | 1.00 32.98 | C |
| ATOM | 491 | NZ | | A1064 | 13.566 | 9.195 | 18.410 | 1.00 35.52 | N |
| ATOM | 492 | C | | A1064 | 20.845 | 10.907 | 18.949 | 1.00 22.52 | C |
| ATOM | 493 | Ö | | A1064 | 21.285 | 10.572 | 20.047 | 1.00 21.41 | Ö |
| ATOM | 494 | N | | A1065 | 21.539 | 10.774 | 17.820 | 1.00 21.47 | N |
| ATOM | 495 | CA | | A1065 | 22.885 | 10.220 | 17.826 | 1.00 22.53 | C |
| ATOM | 496 | CB | | A1065 | 23.379 | 9.980 | 16.399 | 1.00 20.33 | č |
| ATOM | 497 | C | | A1065 | 23.796 | 11.207 | 18.537 | 1.00 24.41 | c |
| MOTA | 498 | 0 | | A1065 | 24.751 | 10.811 | 19.201 | 1.00 24.41 | Ö |
| ATOM | 499 | N | | A1066 | 23.499 | 12.496 | 18.390 | 1.00 24.00 | N |
| ATOM | 500 | CA | | A1066 | 24.283 | 13.530 | 19.049 | 1.00 20.03 | C |
| ATOM | 501 | CB | | A1066 | 24.167 | 14.859 | 18.309 | 1.00 34.23 | C |
| ATOM | 502 | | | A1066 | 24.913 | 14.895 | 16.997 | 1.00 40.28 | C |
| | 503 | CG | | | | 16.574 | 16.602 | 1.00 48.25 | s |
| ATOM | | SD | | A1066 A1066 | 25.423 | | | 1.00 46.23 | C |
| ATOM | 504 | CE | | | 27.174 | 16.492 13.716 | 17.024 | 1.00 48.99 | C |
| ATOM | 505 | C | | A1066 | 23.826 | | 20.493 | | |
| ATOM | 506 | 0 | | A1066 | 24.456 22.720 | 14.443 | 21.254 20.856 | 1.00 33.60 1.00 33.56 | O N |
| ATOM | 507 | N | | A1067 | | 13.069 | | | C |
| ATOM | 508 | CA | | A1067 | 22.217 | 13.159 | 22.216 | 1.00 34.99 | C |
| ATOM | 509 | C | | A1067 | 21.311 21.237 | 14.339 14.787 | 22.519 23.666 | 1.00 36.72 1.00 34.92 | 0 |
| ATOM | 510 | 0 | | A1067 | 20.616 | 14.845 | 21.504 | 1.00 34.92 | N |
| ATOM | 511 | N | | A1068 | | | | 1.00 39.81 | C |
| ATOM | 512 | CA | | A1068 | 19.716 | 15.975 17.316 | 21.699 21.504 | 1.00 39.81 | C |
| ATOM | 513 | CB | | A1068 | 20.455 | | | 1.00 40.09 | 0 |
| ATOM | 514 | OG1 | | A1068 | 19.535 | 18.400 17.396 | 21.687 20.114 | 1.00 42.07 | C |
| MOTA | 515 | | | A1068 | 21.062 18.520 | 15.922 | 20.752 | 1.00 40.32 | C |
| ATOM | 516 | C | | A1068 | | 14.915 | 20.732 | 1.00 40.02 | 0 |
| ATOM | 517 | O N | | A1068 A1069 | 18.293 17.753 | 17.007 | 20.716 | 1.00 41.29 | И |
| ATOM ATOM | 518 519 | CA | | A1069 | 16.586 | 17.061 | 19.856 | 1.00 40.01 | C |
| ATOM | 520 | C | | A1069 | 16.835 | 17.849 | 18.587 | 1.00 40.96 | c |
| | 521 | 0 | | A1069 | 17.705 | 18.722 | 18.547 | 1.00 40.30 | Ö |
| MOTA | 522 | N | | A1009 | 16.065 | 17.545 | 17.547 | 1.00 40.13 | N |
| ATOM | 523 | CA | | A1070 | 16.207 | 18.224 | | | ć |
| ATOM | | | | | 15.288 | 17.591 | 15.200 | 1.00 40.90 | C |
| ATOM ATOM | 524 | CB | | A1070 A1070 | 13.828 | 17.774 | 15.593 | 1.00 40.70 | C |
| | 525 526 | | | A1070 | 15.557 | 18.227 | 13.835 | 1.00 40.33 | C |
| ATOM | 527 | | | A1070 | 16.980 | 18.055 | 13.352 | 1.00 41.45 | , C |
| ATOM ATOM | 528 | CDI | | A1070 | 15.876 | 19.712 | 16.387 | 1.00 39.83 | C |
| ATOM | 529 | 0 | | A1070 | 16.354 | 20.533 | 15.598 | 1.00 41.49 | 0 |
| ATOM | 530 | N | | A1070 A1071 | 15.058 | 20.553 | 17.379 | 1.00 41.31 | . и |
| ATOM | 531 | CA | | A1071 | 14.672 | 21.442 | 17.594 | 1.00 42.83 | C |
| ATOM | 532 | CB | | A1071 | 13.546 | 21.531 | 18.633 | 1.00 42.83 | C |
| ATOM | 533 | OG | | A1071 | 13.938 | 20.980 | 19.877 | 1.00 44.55 | 0 |
| ATOM | 534 | C | | A1071 | 15.856 | 22.295 | 18.039 | 1.00 44.33 | Č |
| 121012 | J J 4 | _ | ∕انتان | 77011 | 13.036 | 24.293 | 10.039 | 1.00 43.32 | C |

| ATOM | 535 | 0 | SER | A1071 | 15.79 | 2 23.523 | 17.984 | 1.00 44.46 | 0 |
|------|-----|--------|-----|-------|-------|-----------|--------|------------|---|
| ATOM | 536 | N | | A1072 | 16.93 | | 18.472 | 1.00 42.56 | N |
| ATOM | 537 | CA | | A1072 | 18.12 | | 18.911 | 1.00 41.56 | c |
| ATOM | 538 | СВ | | A1072 | 18.74 | | 20.141 | 1.00 41.25 | C |
| ATOM | 539 | CG | | A1072 | 19.60 | | 19.844 | 0.05 41.20 | Č |
| ATOM | 540 | CD | | A1072 | 21.06 | | 19.724 | 0.05 41.09 | Č |
| ATOM | 541 | CE | | A1072 | 21.60 | | 21.037 | 0.05 41.03 | c |
| | | | | | | | | | |
| ATOM | 542 | NZ | | A1072 | 21.47 | | 22.152 | 0.05 40.94 | N |
| ATOM | 543 | C | | A1072 | 19.13 | | 17.777 | 1.00 41.40 | C |
| MOTA | 544 | 0 | | A1072 | 19.84 | | 17.643 | 1.00 41.76 | 0 |
| MOTA | 545 | N | | A1073 | 19.22 | | 16.960 | 1.00 40.37 | Ŋ |
| ATOM | 546 | CA | | A1073 | 20.14 | • | 15.829 | 1.00 38.42 | C |
| ATOM | 547 | CB | | A1073 | 20.43 | | 15.339 | 1.00 39.84 | С |
| ATOM | 548 | CG | | A1073 | 21.48 | 9 19.100 | 16.015 | 1.00 40.56 | С |
| MOTA | 549 | CD1 | LEU | A1073 | 22.58 | 5 19.956 | 16.635 | 1,00 41.19 | С |
| ATOM | 550 | CD2 | LEU | A1073 | 20.82 | 0 18.243 | 17.064 | 1.00 42.23 | C |
| ATOM | 551 | С | LEU | A1073 | 19.55 | 6 22.198 | 14.664 | 1.00 36.59 | C |
| ATOM | 552 | 0 | LEU | A1073 | 20.20 | 5 23.091 | 14.123 | 1.00 36.83 | 0 |
| ATOM | 553 | N | GLY | A1074 | 18.32 | 6 21.849 | 14.285 | 1.00 34.67 | N |
| ATOM | 554 | CA | GLY | A1074 | 17.65 | | 13.172 | 1.00 31.12 | С |
| ATOM | 555 | С | | A1074 | 17.74 | | 11.927 | 1.00 29.81 | С |
| ATOM | 556 | Ó | | A1074 | 18.83 | | 11.576 | 1.00 29.20 | 0 |
| ATOM | 557 | N | | A1075 | 16.61 | | 11.260 | 1.00 29.29 | N |
| ATOM | 558 | CA | | A1075 | 16.59 | | 10.051 | 1.00 29.15 | c |
| ATOM | 559 | CB | | A1075 | 15.16 | | 9.502 | 1.00 28.80 | c |
| | 560 | CG | | A1075 | 14.24 | | 10.353 | 1.00 20.00 | Č |
| ATOM | | | | | | | | 1.00 29.16 | c |
| ATOM | 561 | | | A1075 | 13.30 | | 11.183 | | |
| ATOM | 562 | | | A1075 | 14.30 | | 10.315 | 1.00 28.39 | C |
| ATOM | 563 | | | A1075 | 12.44 | | 11.964 | 1.00 28.84 | C |
| MOTA | 564 | | | A1075 | 13.45 | | 11.089 | 1.00 30.94 | C |
| MOTA | 565 | CZ | | A1075 | 12.51 | | | 1.00 29.27 | C |
| ATOM | 566 | С | | A1075 | 17.50 | | 8.922 | 1.00 29.25 | С |
| MOTA | 567 | 0 | | A1075 | 18.09 | | 8.193 | 1.00 27.78 | 0 |
| MOTA | 568 | N | GLN | A1076 | 17.58 | 9 22.393 | | 1.00 29.64 | N |
| ATOM | 569 | CA | GLN | A1076 | 18.39 | 7 23.008 | 7.717 | 1.00 29.73 | С |
| MOTA | 570 | CB | GLN | A1076 | 18.04 | 6 24.497 | 7.593 | 1.00 31.55 | С |
| ATOM | 571 | CG | GLN | A1076 | 16.58 | 5 24.746 | 7.253 | 1.00 31.77 | С |
| MOTA | 572 | CD | GLN | A1076 | 16.20 | 2 24.181 | 5.895 | 1.00 32.15 | С |
| MOTA | 573 | OE1 | GLN | A1076 | 15.04 | 4 23.849 | 5.652 | 1.00 34.09 | 0 |
| ATOM | 574 | NE2 | GLN | A1076 | 17.17 | 4 24.084 | 5.002 | 1.00 32.35 | N |
| ATOM | 575 | С | GLN | A1076 | 19.88 | 8 22.845 | 7.975 | 1.00 31.01 | С |
| MOTA | 576 | 0 | GLN | A1076 | 20.72 | | 7.099 | 1.00 30.59 | 0 |
| MOTA | 577 | N | ASP | A1077 | 20.21 | | | 1.00 30.30 | N |
| ATOM | 578 | CA | | A1077 | 21.59 | | | 1.00 30.99 | C |
| ATOM | 579 | СВ | | A1077 | 21.68 | | | 1.00 34.42 | Ċ |
| MOTA | 580 | CG | | A1077 | 22.89 | | | | Ċ |
| ATOM | 581 | | | A1077 | 24.02 | | | 1.00 40.63 | ō |
| ATOM | 582 | | | A1077 | 22.71 | | | 1.00 41.18 | Ō |
| ATOM | 583 | C | | A1077 | 22.06 | | | 1.00 28.98 | Č |
| | | | | | | | | 1.00 27.03 | Ö |
| ATOM | 584 | O N | | A1077 | 23.24 | | | | |
| ATOM | 585 | | | A1078 | 21.13 | | | 1.00 26.47 | N |
| ATOM | 586 | CA | | A1078 | 21.47 | | | 1.00 25.11 | С |
| ATOM | 587 | CB | | A1078 | 20.78 | | | 1.00 25.83 | C |
| ATOM | 588 | CG | | A1078 | 21:06 | | | 1.00 25.61 | C |
| MOTA | 589 | | | A1078 | 20.07 | | | 1.00 26.16 | C |
| ATOM | 590 | | | A1078 | 22.49 | | | 1.00 26.52 | C |
| MOTA | 591 | С | LEU | A1078 | 21.01 | .5 18.495 | 6.723 | 1.00 24.62 | С |

| | | | | | • | | | | |
|------|-----|-----|-----|---------|--------|--------|--------|------------|---|
| ATOM | 592 | 0 | LEU | A1078 | 20.052 | 19.125 | 6.296 | 1.00 25.13 | 0 |
| ATOM | 593 | N | GLU | A1079 | 21.710 | 17.648 | 5.975 | 1.00 23.38 | N |
| ATOM | 594 | CA | GLU | A1079 | 21.312 | 17.388 | 4.603 | 1.00 22.76 | С |
| ATOM | 595 | СВ | GLU | A1079 | 22.008 | 18.338 | 3.639 | 1.00 24.57 | C |
| ATOM | 596 | CG | GLU | A1079 | 21.425 | 18.299 | 2.241 | 1.00 25.55 | C |
| ATOM | 597 | CD | GLU | A1079 | 22.219 | 19.146 | 1.274 | 1.00 28.95 | C |
| ATOM | 598 | OE1 | GLU | A1079 | 23.415 | 18.844 | 1.074 | 1.00 28.46 | 0 |
| ATOM | 599 | | | A1079 | 21.652 | 20.114 | 0.722 | 1.00 31.06 | 0 |
| ATOM | 600 | С | | A1079 | 21.639 | 15.958 | 4.220 | 1.00 21.67 | С |
| ATOM | 601 | 0 | GLU | A1079 | 22.747 | 15.476 | 4.458 | 1.00 21.79 | 0 |
| ATOM | 602 | N | VAL | A1080 | 20.667 | 15.283 | 3.626 | 1.00 18.92 | N |
| ATOM | 603 | CA | | A1080 | 20.861 | 13.904 | 3.208 | 1.00 19.27 | С |
| ATOM | 604 | CB | VAL | A1080 | 19.836 | 12.967 | 3.881 | 1.00 18.84 | С |
| ATOM | 605 | | VAL | A1080 | 20.181 | 11.504 | 3.578 | 1.00 18.64 | С |
| ATOM | 606 | | | A1080 | 19.801 | 13.230 | 5.368 | 1.00 18.66 | С |
| ATOM | 607 | С | | A1080 | 20.690 | 13.798 | 1.696 | 1.00 19.85 | C |
| ATOM | 608 | Ō | | A1080 | 19.596 | 14.003 | 1.169 | 1.00 19.06 | 0 |
| ATOM | 609 | N | | A1081 | 21.780 | 13.497 | 1.003 | 1.00 19.76 | N |
| ATOM | 610 | CA | | A1081 | 21.742 | 13.332 | -0.442 | 1.00 20.15 | С |
| ATOM | 611 | CB | | A1081 | 22.808 | 14.210 | -1.111 | 1.00 19.63 | С |
| ATOM | 612 | CG | | A1081 | 22.640 | 15.717 | -0.878 | 1.00 19.82 | C |
| ATOM | 613 | | | A1081 | 23.817 | 16.488 | -1.475 | 1.00 19.43 | С |
| ATOM | 614 | | | A1081 | 21.326 | 16.171 | -1.485 | 1.00 18.80 | С |
| ATOM | 615 | C | | A1081 | 22.037 | 11.861 | -0.696 | 1.00 20.78 | С |
| ATOM | 616 | Õ | | A1081 | 22.097 | 11.067 | 0.242 | 1.00 19.52 | 0 |
| ATOM | 617 | N | | A1082 | 22.224 | 11.495 | -1.957 | 1.00 21.64 | N |
| ATOM | 618 | CA | | A1082 | 22.521 | 10.110 | -2.301 | 1.00 22.51 | С |
| ATOM | 619 | CB | | A1082 | 21.430 | 9.574 | -3.230 | 1.00 21.83 | С |
| ATOM | 620 | CG | | A1082 | 20.134 | 9.281 | -2.485 | 1.00 24.97 | С |
| ATOM | 621 | | | A1082 | 19.930 | 8.174 | -1.973 | 1.00 26.72 | 0 |
| ATOM | 622 | | | A1082 | 19.264 | 10.275 | -2.402 | 1.00 23.64 | N |
| ATOM | 623 | C | | A1082 | 23.897 | 10.029 | -2.954 | 1.00 22.59 | С |
| ATOM | 624 | Ö | | 1 A1082 | 24.196 | 10.786 | -3.876 | 1.00 23.10 | 0 |
| ATOM | 625 | N | | 1 A1083 | 24.738 | 9.118 | -2.472 | 1.00 21.81 | N |
| ATOM | 626 | CA | | N A1083 | 26.079 | 8.998 | -3.021 | 1.00 24.05 | С |
| MOTA | 627 | CB | | N A1083 | 27.011 | 8.298 | -2.018 | 1.00 21.32 | С |
| ATOM | 628 | CG | | N A1083 | 26.634 | 6.849 | -1.748 | 1.00 23.86 | С |
| ATOM | 629 | | | N A1083 | 27.083 | 6.269 | -0.752 | 1.00 23.67 | 0 |
| ATOM | 630 | | | N A1083 | 25.835 | 6.249 | -2.631 | 1.00 20.56 | N |
| MOTA | 631 | C | | N A1083 | 26.112 | 8.315 | -4.385 | 1.00 26.50 | С |
| ATOM | 632 | ō | | N A1083 | 25.065 | 7.986 | -4.951 | 1.00 25.00 | 0 |
| ATOM | 633 | N | | U A1084 | 27.313 | 8.118 | -4.921 | 1.00 28.34 | N |
| ATOM | 634 | CA | | U A1084 | 27.447 | 7.514 | -6.237 | 1.00 32.10 | C |
| ATOM | 635 | CB | | U A1084 | 28.907 | 7.561 | -6.700 | 1.00 32.77 | С |
| ATOM | 636 | | | U A1084 | 29.885 | 6.749 | -5.877 | 1.00 35.30 | С |
| ATOM | 637 | CD | | U A1084 | 31.327 | 7.041 | -6.263 | 1.00 38.54 | С |
| ATOM | 638 | | | U A1084 | 31.628 | -7.058 | -7.478 | 1.00 39.35 | 0 |
| ATOM | 639 | | | U A1084 | 32.160 | 7:252 | -5.356 | 1.00 40.56 | 0 |
| ATOM | 640 | | | U A1084 | 26.906 | 6.092 | -6.307 | | С |
| ATOM | 641 | | | U A1084 | 26.582 | 5.610 | -7.386 | 1.00 34.17 | 0 |
| ATOM | 642 | | | G A1085 | 26.811 | | -5.158 | | N |
| ATOM | 643 | | | G A1085 | 26.278 | 4.069 | -5.111 | | C |
| MOTA | 644 | | | G A1085 | 26.967 | 3.259 | -4.009 | | C |
| ATOM | 645 | | | G A1085 | 28.442 | 2.992 | -4.269 | | C |
| ATOM | 646 | | | G A1085 | 28.668 | 2.173 | -5.540 | | C |
| ATOM | 647 | | | G A1085 | 28.539 | 0.730 | | | N |
| MOTA | 648 | | | G A1085 | 27.396 | | -5.107 | 0.05 30.07 | С |
| | | | | | | | | | |

| | | | | | | | | 0 05 20 16 | N7 |
|--------------|------------|----|-----|----------------|------------------|------------------|----------------|--------------------------|--------|
| ATOM | 649 | | | A1085 | 26.249 | | -5.054 | 0.05 30.16 | N N |
| MOTA | 650 | | | A1085 | | | -4.938 | 0.05 30.04 | C |
| ATOM | 651 | C | ARG | A1085 | 24.768 | | -4.860 | 1.00 28.84 | 0 |
| ATOM | 652 | | | A1085 | 24.121 | | -4.683 | 1.00 28.73 1.00 26.09 | Ŋ |
| MOTA | 653 | | | A1086 | 24.222 | 5.329 | -4.842 | 1.00 24.49 | C |
| MOTA | 654 | | | A1086 | 22.797 | 5.514 | -4.635 | 1.00 24.49 | c |
| MOTA | 655 | | | A1086 | 22.286 | 5.493 | -3.202 | 1.00 25.43 | 0 |
| ATOM | 656 | - | | A1086 | 21.090 | 5.649 | -2.975 | 1.00 23.43 | Ŋ |
| MOTA | 657 | | | A1087 | 23.172 | 5.306 | -2.233 | 1.00 21.30 | C |
| ATOM | 658 | | | A1087 | 22.755 | 5.259 | -0.836 | 1.00 21.27 | c |
| ATOM | 659 | | | A1087 | 23.704 | 4.379 | -0.042 | 1.00 21.23 | Č |
| MOTA | 660 | - | | A1087 | 22.689 | 6.653 | -0.205 | 1.00 21.03 | o |
| ATOM | 661 | _ | | A1087 | 23.508 | 7.529 | -0.499 | 1.00 19.21 | N |
| ATOM | 662 | | | A1088 | 21.700 | 6.872 | 0.668 | 1.00 20.00 | C |
| ATOM | 663 | | | A1088 | 20.666 | 5.919 | 1.105 1.335 | 1.00 20.18 | Ċ |
| ATOM | 664 | CA | | A1088 | 21.544 | 8.164 | | 1.00 20.15 | Ċ |
| ATOM | 665 | CB | | A1088 | 20.212 | 8.013 | 2.064 2.390 | 1.00 20.83 | č |
| MOTA | 666 | CG | | A1088 | 20.183 | 6.545 | 2.281 | 1.00 19.50 | č |
| MOTA | 667 | С | | A1088 | 22.714 | 8.380 | 2.281 | 1.00 17.61 | Ö |
| ATOM | 668 | 0 | | A1088 | 23.220 | 7.431 | 2.395 | 1.00 17.01 | N |
| MOTA | 669 | N | | A1089 | 23.164 | 9.621 9.913 | 3.279 | 1.00 19.12 | . C |
| MOTA | 670 | CA | | A1089 | 24.281 | 9.913 | 2.557 | 1.00 20.66 | Č |
| ATOM | 671 | СВ | | A1089 | 25.611 | 10.698 | 1.534 | 1.00 23.33 | č |
| ATOM | 672 | CG | | A1089 | 25.977 | 11.724 | 1.853 | 1.00 22.08 | Č |
| MOTA | 673 | | | A1089 | 26.869 | 12.699 | 0.916 | 1.00 22.82 | č |
| MOTA | 674 | | | A1089 | 27.211 | | 0.249 | 1.00 22.30 | Č |
| MOTA | 675 | | | A1089 | 25.426 | 10.673 11.642 | -0.692 | 1.00 22.30 | č |
| ATOM | 676 | | | A1089 | 25.752 | | -0.354 | 1.00 25.15 | č |
| ATOM | 677 | CZ | | A1089 | 26.649 | 12.655 13.614 | -1.288 | 1.00 24.63 | ő |
| ATOM | 678 | OH | | A1089 | 26.987 24.205 | 11.363 | 3.699 | 1.00 17.64 | Ċ |
| ATOM | 679 | C | | A1089 | 23.578 | 12.178 | 3.023 | 1.00 16.44 | 0 |
| MOTA | 680 | 0 | | A1089 | 24.824 | 11.691 | 4.825 | 1.00 17.81 | N |
| ATOM | 681 | N | | A1090 A1090 | 24.801 | 13.070 | 5.277 | 1.00 17.81 | С |
| MOTA | 682 | CA | | | 25.019 | 13.159 | 6.791 | 1.00 17.48 | С |
| ATOM | 683 | CB | | A1090 A1090 | 23.777 | 12.873 | 7.595 | 1.00 17.01 | C |
| ATOM | 684 | CG | | A1090 | 23.434 | 11.568 | 7.938 | 1.00 17.02 | С |
| ATOM | 685 | | | A1090 | 22.919 | 13.910 | 7.962 | 1.00 16.23 | С |
| ATOM | 686 | | | A1090 | 22.247 | 11.293 | 8.632 | 1.00 17.95 | С |
| ATOM | 687 688 | | | A1090 | 21.732 | 13.647 | 8.656 | 1.00 17.65 | С |
| ATOM | 689 | CZ | | A1090 | 21.397 | 12.333 | 8.989 | 1.00 16.73 | С |
| MOTA MOTA | 690 | C | | A1090 | 25.852 | 13.892 | 4.547 | 1.00 20.29 | С |
| ATOM | 691 | Ö | _ | A1090 | 27.054 | 13.713 | 4.749 | 1.00 19.58 | 0 |
| ATOM | 692 | N | | R A1091 | 25.384 | 14.767 | 3.665 | 1.00 21.20 | N |
| ATOM | 693 | CA | | R A1091 | 26.266 | 15.646 | 2.921 | 1.00 23.08 | С |
| ATOM | 694 | СВ | | R A1091 | 25.592 | 16.086 | 1.618 | 1.00 24.12 | С |
| ATOM | 695 | OG | | R A1091 | 24.281 | 16.567 | 1.852 | 1.00 24.36 | , 0 |
| ATOM | 696 | C | | R A1091 | 26.580 | 16.856 | 3.806 | | С |
| ATOM | 697 | | | R A1091 | 27.613 | 17.507 | 3.642 | 1.00 25.24 | 0 |
| MOTA | 698 | | | N A1092 | 25.685 | 17.141 | 4.752 | 1.00 24.80 | N |
| ATOM | 699 | | | N A1092 | 25.853 | 18.254 | 5.688 | 1.00 24.09 | С |
| MOTA | 700 | | | N A1092 | 24.970 | 19.448 | 5.296 | 1.00 26.54 | C |
| ATOM | 701 | | | N A1092 | 25.294 | 20.132 | | | С |
| ATOM | 702 | | | N A1092 | 26.711 | 20.678 | 3.907 | | |
| ATOM | 703 | | | N A1092 | 27.257 | 21.147 | | | |
| ATOM | 704 | | | N A1092 | 27.308 | | | | |
| ATOM | 705 | | GL | N A1092 | 25.453 | 17.803 | 7.096 | 1.00 23.97 | С |
| | | | | | | | | | |

| ATOM | 706 | 0 | GLN | A1092 | 24.343 | 17.295 | 7.300 | 1.00 22.36 | 0 |
|--------------|--------------------|---------|-----|--------------------|------------------|------------------|------------------|--------------------------|---|
| ATOM | 707 | | ALA | A1093 | 26.356 | 17.989 | 8.057 | 1.00 20.55 | N |
| MOTA | 708 | CA . | ALA | A1093 | 26.097 | 17.621 | 9.447 | 1.00 21.00 | C |
| MOTA | 709 | CB . | ALA | A1093 | 25.948 | 16.101 | 9.580 | 1.00 17.57 | C |
| MOTA | 710 | C | ALA | A1093 | 27.235 | | 10.336 | 1.00 22.11 | C |
| MOTA | 711 | 0 | ALA | A1093 | 28.392 | 18.120 | 9.920 | 1.00 23.23 | 0 |
| MOTA | 712 | N | PRO | A1094 | 26.918 | | 11.573 | 1.00 23.31 | N |
| MOTA | 713 | CD | PRO | A1094 | 25.550 | | 12.111 | 1.00 23.07 | C |
| ATOM | 714 | CA | PRO | A1094 | 27.907 | | 12.533 | 1.00 24.58 | C |
| ATOM | 715 | CB | PRO | A1094 | 27.053 | | 13.521 | 1.00 24.45 | C |
| ATOM | 716 | | | A1094 | 25.798 | | 13.575 | 1.00 24.77 | c |
| ATOM | 717 | | | A1094 | 28.687 | | 13.219 | 1.00 26.12 | 0 |
| MOTA | 718 | 0 | | A1094 | 28.675 | 17.791 | 14.445 | 1.00 27.56 1.00 26.05 | И |
| MOTA | 719 | N | | A1095 | 29.353 | 17.079 | 12.423 | 1.00 26.03 | c |
| MOTA | 720 | CA | | A1095 | 30.139 | 15.975 | 12.957 | 1.00 27.36 | c |
| ATOM | 721 | CB | | A1095 | 29.279 | 14.710 | 13.090 13.674 | 1.00 26.42 | č |
| MOTA | 722 | CG | | A1095 | 30.016 | 13.544 | 12.931 | 1.00 26.59 | Ċ |
| MOTA | 723 | | | A1095 | 30.208 | 12.385 | 14.950 | 1.00 27.10 | c |
| MOTA | 724 | | | A1095 | 30.571 30.946 | 13.625 11.324 | 13.446 | 1.00 26.29 | Ċ |
| MOTA | 725 | | | A1095 | 30.946 | 12.574 | 15.475 | 1.00 25.68 | č |
| ATOM | 726 | | | A1095 | 31.502 | 11.417 | 14.720 | 1.00 27.52 | Ċ |
| ATOM | 727 | CZ | | A1095 A1095 | 31.305 | 15.727 | 12.012 | 1.00 26.40 | С |
| ATOM | 728 | C | | | 31.122 | 15.681 | 10.792 | 1.00 25.80 | 0 |
| ATOM | 729 | O NI | | A1095 A1096 | 32.498 | 15.560 | 12.577 | 1.00 26.14 | N |
| ATOM | 730 | N CA | | A1096 | 33.705 | 15.357 | 11.781 | 1.00 29.05 | С |
| MOTA | 731 732 | CB | | A1096 | 34.909 | 15.969 | 12.500 | 1.00 30.71 | С |
| MOTA MOTA | 733 | OG | | A1096 | 34.768 | 17.373 | 12.603 | 1.00 37.13 | 0 |
| ATOM | 734 | C | - | A1096 | 34.039 | 13.919 | 11.413 | 1.00 28.85 | C |
| ATOM | 735 | 0 | | A1096 | 34.702 | 13.678 | 10.407 | 1.00 29.54 | 0 |
| ATOM | 736 | N | | A1097 | 33.595 | 12.968 | 12.229 | 1.00 28.58 | N |
| ATOM | 737 | CA | | A1097 | 33.888 | 11.573 | 11.957 | 1.00 27.16 | С |
| ATOM | 738 | C | | A1097 | 32.991 | 10.948 | 10.907 | 1.00 26.54 | С |
| ATOM | 739 | Ō | | A1097 | 32.406 | 11.648 | 10.077 | 1.00 27.09 | 0 |
| ATOM | 740 | N | LYS | A1098 | 32.888 | 9.624 | 10.931 | 1.00 24.94 | N |
| MOTA | 741 | CA | LYS | A1098 | 32.045 | 8.930 | 9.973 | 1.00 25.69 | C |
| ATOM | 742 | CB | LYS | A1098 | 32.587 | 7.535 | 9.644 | 1.00 29.36 | C |
| MOTA | 743 | CG | LYS | A1098 | 33.687 | 7.015 | 10.547 | 1.00 33.98 | C |
| MOTA | 744 | CD | LYS | S A1098 | 35.051 | 7.532 | 10.120 | 1.00 37.43 | C |
| MOTA | 745 | CE | LYS | 5 A1098 | 36.164 | 6.583 | 10.568 | 1.00 39.11 | N |
| MOTA | 746 | NZ | | S A1098 | 36.119 | 6.320 | 12.033 | 1.00 41.00 | C |
| MOTA | 747 | C | | S A1098 | 30.625 | 8.796 | 10.492 | 1.00 24.62 1.00 22.63 | 0 |
| MOTA | 748 | 0 | | S A1098 | 30.393 | 8.494 | 11.668 | 1.00 22.03 | N |
| ATOM | 749 | N | | E A1099 | 29.677 | 9.033 8.932 | 9.600 9.941 | 1.00 21.57 | c |
| ATOM | 750 | | | E A1099 | 28.273 | - | 9.523 | | Č |
| ATOM | 751 | CB | | E A1099 | 27.514 | 10.193 10.056 | 9.905 | | Ċ |
| MOTA | 752 | | | E A1099 | 26.039 28.155 | 11:419 | 10.177 | | C |
| MOTA | 753 | | | E A1099 | 27.677 | 12.738 | 9.613 | | С |
| ATOM | 754 | | | E A1099 | 27.695 | 7.748 | 9.184 | | С |
| ATOM | 755 | | | E A1099 E A1099 | 27.597 | 7.775 | 7.958 | | 0 |
| ATOM | 756 75 7 | | | P A1100 | 27.334 | 6.699 | 9.907 | | N |
| ATOM | 758 | | | P A1100 | 26.760 | | 9.270 | | C |
| ATOM | 759 | | | P A1100 | 27.172 | | 10.009 | | С |
| ATOM ATOM | 760 | | | P A1100 | 28.652 | | 9.945 | 1.00 19.33 | С |
| ATOM | 761 | CD: | | P A1100 | 29.370 | | | | С |
| ATOM | 762 | | | P A1100 | 30.743 | | | _ | С |
| ALON | , 52 | | • | | | | | | |

| ATOM | 763 | CE3 | TRP A1100 | 28.987 | 2.835 | 7.634 | 1.00 19.76 | C |
|--------------|------------|-------|------------------|--------|----------------|----------------|--------------------------|--------|
| MOTA | 764 | CD1 | TRP A1100 | 29.590 | 4.362 | 10.873 | 1.00 19.35 | C |
| MOTA | 765 | | TRP A1100 | 30.846 | 4.010 | 10.439 | 1.00 18.87 | N |
| ATOM | 766 | CZ2 | TRP A1100 | 31.739 | 2.895 | 8.369 | 1.00 19.48 | C |
| ATOM | 767 | CZ3 ' | TRP A1100 | 29.978 | 2.317 | 6.796 | 1.00 22.42 | C |
| MOTA | 768 | CH2 ' | TRP A1100 | 31.343 | 2.354 | 7.172 | 1.00 20.56 | C |
| ATOM | 769 | C ' | TRP A1100 | 25.251 | 5.718 | 9.294 | 1.00 20.31 | С |
| ATOM | 770 | 0 ' | TRP A1100 | 24.633 | 5.795 | 10.357 | 1.00 20.18 | 0 |
| ATOM | 771 | N | LEU A1101 | 24.663 | 5.829 | 8.113 | 1.00 18.06 | N |
| MOTA | 772 | CA | LEU A1101 | 23.229 | 6.023 | 8.019 | 1.00 17.46 | C |
| ATOM | 773 | CB | LEU A1101 | 22.915 | 7.399 | 7.409 | 1.00 15.91 | C |
| ATOM | 774 | CG | LEU A1101 | 21.475 | 7.611 | 6.919 | 1.00 15.54 | C |
| MOTA | 775 | | LEU A1101 | 20.510 | 7.621 | 8.101 | 1.00 14.01 | С |
| MOTA | 776 | CD2 | LEU A1101 | 21.380 | 8.931 | 6.150 | 1.00 12.69 | С |
| ATOM | 777 | С | LEU A1101 | 22.561 | 4.945 | 7.190 | 1.00 17.42 | С |
| ATOM | 778 | 0 | LEU A1101 | 23.124 | 4.436 | 6.218 | 1.00 15.25 | 0 |
| ATOM | 779 | N | SER A1102 | 21.353 | 4.582 | 7.600 | 1.00 17.54 | N |
| ATOM | 780 | CA | SER A1102 | 20.581 | 3.607 | 6.865 | 1.00 15.75 | C |
| MOTA | 781 | CB | SER A1102 | 20.832 | 2.189 | 7.364 | 1.00 16.41 | C |
| ATOM | 782 | OG | SER A1102 | 20.242 | 1.258 | 6.469 | 1.00 14.51 | 0 |
| MOTA | 783 | С | SER A1102 | 19.129 | 3.980 | 7.063 | 1.00 17.48 | С |
| MOTA | 784 | 0 | SER A1102 | 18.711 | 4.322 | 8.173 | 1.00 16.20 | 0 |
| ATOM | 785 | N | ILE A1103 | | | 5.968 | 1.00 17.02 | N |
| MOTA | 786 | CA | ILE A1103 | | 4.274 | 5.979 | 1.00 17.85 | C |
| MOTA | 787 | CB | ILE A1103 | | 5.576 | 5.194 | 1.00 19.00 | C C |
| ATOM | 788 | | ILE A1103 | | 5.948 | 5.278 | 1.00 18.57 | |
| ATOM | 789 | | ILE A1103 | | 6.706 | 5.754 | 1.00 18.22 | c c |
| ATOM | 790 | | ILE A1103 | | 8.014 | 4.999 | 1.00 20.97 | C |
| MOTA | 791 | С | ILE A1103 | | | 5.291 | 1.00 17.46 | |
| MOTA | 792 | 0 | ILE A1103 | | 2.510 | 4.368 | 1.00 17.27 | N O |
| MOTA | 793 | N | SER A1104 | | 2.845 | 5.751 | 1.00 14.92 | C |
| ATOM | 794 | CA | SER A1104 | | 1.772 | 5.175 | 1.00 17.06 | c |
| MOTA | 795 | CB | SER A1104 | | 0.447 | 5.876 | 1.00 15.94 | 0 |
| MOTA | 796 | OG | SER A1104 | , | -0.613 | 5.342 | 1.00 15.77 | Ċ |
| MOTA | 797 | С | SER A1104 | | 2.155 | 5.384 | 1.00 17.20 | 0 |
| MOTA | 798 | 0 | SER Allo4 | | 2.859 | 6.333 | 1.00 15.90 1.00 18.52 | N |
| MOTA | 799 | N | HIS A1105 | | 1.699 | 4.502 | | c |
| ATOM | 800 | . CA | HIS A1105 | | 2.048 | 4.619 | 1.00 20.22 1.00 23.50 | č |
| MOTA | 801 | | HIS A1105 | | 3.316 3.127 | 3.813 2.334 | 1.00 25.77 | č |
| ATOM | 802 | CG | HIS A1105 | | 2.690 | 1.392 | 1.00 26.90 | c |
| ATOM | 803 | | HIS A1105 | | 3.301 | 1.687 | 1.00 26.39 | N |
| ATOM | 804 | | HIS A110 | | 2.977 | 0.412 | | c |
| ATOM | 805 | | HIS A110 | | 2.601 | 0.208 | 1.00 27.67 | N |
| ATOM | 806 | | HIS A110 | | 0.953 | 4.079 | | С |
| ATOM | 807 | | HIS Allo | | 0.040 | 3.392 | | 0 |
| ATOM | 808 | | HIS A110 | | -1.067 | | | N |
| ATOM | 809 | | THR Allo | | 0.160 | | | _ |
| ATOM | 810 | | THR AllO | | -0.682 | | | С |
| ATOM ATOM | 811 812 | | THR AIIO | | 0.169 | | | 0 |
| ATOM | 813 | | THR A110 | | -1.415 | | | С |
| ATOM | 814 | | THR AllO | | 1.161 | | | С |
| ATOM | 815 | | THR Allo | | 2.356 | | | 0 |
| ATOM | 816 | | ASP Allo | | 0.698 | | | N |
| ATOM | 817 | | ASP Allo | | 1.612 | | | С |
| ATOM | 818 | | ASP AllO | | 0.845 | | | С |
| ATOM | 819 | | ASP A110 | | 0.098 | | | С |
| ATOM | 011 | | | | | | | |

| ATOM | 820 | OD1 A | ASP A | A1107 | 4.229 | 0.704 | -0.225 | 1.00 | | 0 | |
|------|-----|-------|-------|---------|--------------|---------|----------|------|----------------|---|--------|
| ATOM | 821 | OD2 A | | | 3.134 | -1.093 | 0.413 | 1.00 | | 0 | |
| MOTA | 822 | C P | ASP A | A1107 | 3.420 | 2.385 | 3.691 | 1.00 | | С | |
| ATOM | 823 | O F | ASP A | A1107 | 2.613 | 3.285 | 3.470 | 1.00 | | 0 | |
| ATOM | 824 | N G | GLN A | A1108 | 3.801 | 2.049 | 4.921 | 1.00 | 25.83 | N | |
| ATOM | 825 | | | A1108 | 3.228 | 2.710 | 6.086 | 1.00 | | C | |
| ATOM | 826 | | | A1108 | 2.384 | 1.710 | 6.867 | 1.00 | 27.32 | C | |
| MOTA | 827 | | | A1108 | 1.328 | | 6.030 | 1.00 | 32.60 | C | ; |
| ATOM | 828 | | | A1108 | 0.95 | | 6.583 | 1.00 | 35.93 | C | ; |
| ATOM | 829 | | | A1108 | 1.089 | | 5.902 | 1.00 | 37.52 | C |) |
| ATOM | 830 | | | A1108 | 0.48 | | 7.829 | 1.00 | 36.07 | N | Į |
| ATOM | 831 | | | A1108 | 4.22 | | 7.038 | 1.00 | 24.10 | C | 3 |
| ATOM | 832 | _ | | A1108 | 3.87 | | 7.742 | 1.00 | | C |) |
| | 833 | | | A1109 | 5.44 | | 7.082 | 1.00 | | N | 1 |
| ATOM | 834 | | | A1109 | 6.45 | | 7.983 | 1.00 | | | 3 |
| ATOM | | | | A1109 | 6.71 | | 9.164 | 1.00 | | | 3 |
| ATOM | 835 | | | A1109 | 5.51 | | 10.004 | 1.00 | | | 2 |
| ATOM | 836 | | | A1109 | 4.74 | | 9.763 | | 26.55 | | 2 |
| ATOM | 837 | | | | 5.15 | | 11.044 | | 26.19 | | С |
| ATOM | 838 | | | A1109 | 3.62 | | 10.549 | 1.00 | | | C |
| MOTA | 839 | | | A1109 | | | 11.834 | | 26.65 | | C |
| ATOM | 840 | | | A1109 | 4.03 3.27 | | 11.584 | | 25.88 | | Č |
| ATOM | 841 | | | A1109 | | | | | 20.22 | | Č |
| ATOM | 842 | | | A1109 | 7.78 | | | | 19.27 | | 0 |
| ATOM | 843 | | | A1109 | 8.09 | | | | 18.43 | | N |
| ATOM | 844 | | | A1110 | 8.57 | | | | 19.10 | | C |
| ATOM | 845 | | | A1110 | 9.92 | | | | 19.10 | | C |
| MOTA | 846 | | | A1110 | 10.04 | | | | 19.30 | | c |
| MOTA | 847 | | | A1110 | 9.65 | | | | 23.53 | | C |
| ATOM | 848 | | | A1110 | 11.47 | | | | 19.12 | | C |
| MOTA | 849 | | | A1110 | 10.74 | | | | | | 0 |
| MOTA | 850 | | | A1110 | 10.28 | _ | | | 17.72 18.67 | | N |
| ATOM | 851 | | | A1111 | 11.92 | | | | | | C |
| ATOM | 852 | | | A1111 | 12.80 | | | | 20.42 | | C |
| ATOM | 853 | CB | | A1111 | 12.89 | | | | 22.98 25.86 | | 0 |
| ATOM | 854 | | | A1111 | 13.36 | | | | 24.99 | | С |
| ATOM | 855 | | | A1111 | 11.54 | | | | | | C |
| MOTA | 856 | С | | A1111 | 14.20 | | | | 20.11 20.53 | | 0 |
| MOTA | 857 | 0 | | A1111 | 14.57 | | | | | | N |
| ATOM | 858 | N | | A1112 | 14.96 | | _ | | 17.15 | | C |
| ATOM | 859 | CA | | A1112 | 16.32 | | | | 18.28 | | c |
| MOTA | 860 | CB | | A1112 | 16.35 | | | | 16.81 | | č |
| MOTA | 861 | С | | A1112 | 17.19 | | | | 18.04 | | o |
| ATOM | 862 | 0 | | A1112 | 16.72 | | | | 17.37 17.48 | | N |
| MOTA | 863 | N | | A1113 | 18.4 | | | | | | C |
| MOTA | 864 | CA | _ | A1113 | 19.40 | | 12.146 | | 17.23 | | C |
| MOTA | 865 | CB | | A1113 | 19.6 | | | | 15.09 | | 0 |
| MOTA | 866 | OG | | A1113 | 20.6 | | | | 16.24 | | c |
| MOTA | 867 | С | | A1113 | 20.7 | | | | 17.94 | | 0 |
| ATOM | 868 | 0 | | A1113 | 21.2 | | | | 18.05 | | |
| ATOM | 869 | N | | A1114 | 21.2 | | | | 18.42 | | N C |
| MOTA | 870 | CA | | A1114 | 22.5 | | | | 17.97 | | |
| MOTA | 871 | CB | | A1114 | 22.3 | | | - | 17.35 | | C |
| ATOM | 872 | | | A1114 | 23.7 | | | | 15.58 | | C |
| ATOM | 873 | CG2 | | A1114 | 21.5 | | | | 16.65 | | C |
| MOTA | 874 | | | A1114 | 23.5 | | | | 18.00 | | C |
| MOTA | 875 | 0 | | A1114 | 23.2 | | | | 17.56 | | O N |
| ATOM | 876 | N | ILE | : A1115 | 24.7 | 93 5.88 | 5 13.286 | 7.00 | 17.57 | | N |
| | | | | | | | | | | | |

| ATOM | 877 | CA | | A1115 | 25.885 | 5.536 | 14.181 | 1.00 15.61 | С |
|------|-----|-----|-----|-------|------------------|--------|---------|------------|-----|
| ATOM | 878 | CB | ILE | A1115 | 26.416 | 4.109 | 13.951 | 1.00 17.48 | С |
| ATOM | 879 | CG2 | ILE | A1115 | 27.514 | 3.806 | 14.965 | 1.00 14.97 | С |
| ATOM | 880 | CG1 | ILE | A1115 | 25.287 | 3.086 | 14.082 | 1.00 16.92 | С |
| ATOM | 881 | CD1 | ILE | A1115 | 25.695· | 1.685 | 13.638 | 1.00 16.69 | . С |
| ATOM | 882 | С | | A1115 | 27.019 | 6.499 | 13.860 | 1.00 17.74 | C |
| ATOM | 883 | ō | | A1115 | 27.470 | 6.573 | 12.714 | 1.00 16.21 | Ō |
| ATOM | 884 | N | | A1116 | 27.470 | 7.246 | 14.864 | 1.00 17.78 | N |
| ATOM | 885 | | | A1116 | 28.562 | 8.188 | | 1.00 17.70 | C |
| | | CA | | | | | 14.668 | | |
| ATOM | 886 | CB | | A1116 | 28.333 | 9.442 | 15.510 | 1.00 20.38 | C |
| ATOM | 887 | CG | | A1116 | 26.963 | 10.095 | 15.322 | 1.00 20.47 | C |
| ATOM | 888 | | | A1116 | 26.877 | 11.326 | 16.205 | 1.00 22.94 | c |
| ATOM | 889 | | | A1116 | 26.751 | 10.462 | 13.860 | 1.00 18.60 | С |
| ATOM | 890 | С | LEU | A1116 | 29.851 | 7.490 | 15.093 | 1.00 21.10 | С |
| MOTA | 891 | 0 | LEU | A1116 | 29.909 | 6.870 | 16.156 | 1.00 19.16 | 0 |
| ATOM | 892 | N | GLU | A1117 | 30.880 | 7.590 | 14.259 | 1.00 22.54 | N |
| ATOM | 893 | CA | GLU | A1117 | 32.141 | 6.934 | 14.554 | 1.00 25.40 | С |
| ATOM | 894 | CB | GLU | A1117 | 32.323 | 5.743 | 13.616 | 1.00 25.16 | С |
| ATOM | 895 | CG | GLU | A1117 | 33.629 | 5.000 | 13.817 | 1.00 27.61 | С |
| ATOM | 896 | CD | | A1117 | 33.720 | 3.772 | 12.950 | 1.00 27.04 | С |
| ATOM | 897 | | | A1117 | 33.391 | 3.875 | 11.750 | 1.00 27.90 | 0 |
| ATOM | 898 | | | A1117 | 34.126 | 2.712 | 13.465 | 1.00 27.49 | 0 |
| ATOM | 899 | C | | A1117 | 33.358 | 7.852 | 14.464 | 1.00 27.82 | c |
| ATOM | 900 | ō | | A1117 | 33.425 | 8.742 | 13.616 | 1.00 26.44 | Ö |
| ATOM | 901 | N | | A1118 | 34.328 | 7.605 | 15.339 | 1.00 31.38 | N |
| ATOM | 902 | CA | | A1118 | 35.549 | 8.396 | 15.387 | 1.00 35.38 | c |
| ATOM | 903 | CB | | A1118 | 35.632 | 9.122 | 16.732 | 1.00 38.96 | c |
| ATOM | 904 | CG | | A1118 | 36.450 | 10.397 | 16.732 | 1.00 38.98 | C |
| | 905 | CD | | | | | | 1.00 44.28 | · c |
| ATOM | | | | A1118 | 35.953 36.206 | 11.381 | 15.671 | | 0 |
| ATOM | 906 | | | A1118 | | 11.153 | 14.469 | 1.00 47.99 | |
| ATOM | 907 | | | A1118 | 35.302 | 12.377 | 16.054 | 1.00 49.20 | 0 |
| ATOM | 908 | C | | A1118 | 36.756 | 7.482 | 15.210 | 1.00 36.85 | С |
| ATOM | 909 | 0 | | A1118 | 37.586 | 7.767 | 14.319 | 1.00 39.18 | 0 |
| ATOM | 910 | OXT | | A1118 | 36.858 | 6.488 | 15.967 | 1.00 37.85 | 0 |
| TER | 911 | | | A1118 | | | | | _ |
| ATOM | 912 | CB | | B2003 | 36.089 | -4.001 | 20.131 | 1.00 36.93 | C |
| ATOM | 913 | CG | | B2003 | 35.997 | -4.450 | 21.581 | 1.00 42.07 | C |
| ATOM | 914 | SD | | B2003 | 37.062 | -5.865 | 21.964. | | S |
| ATOM | 915 | CE | | B2003 | 36.267 | -7.158 | 21.006 | 1.00 46.76 | С |
| ATOM | 916 | С | | B2003 | 33.796 | -3.017 | 20.233 | 1.00 31.67 | C |
| ATOM | 917 | 0 | | B2003 | 33.469 | -2.921 | 21.422 | 1.00 28.54 | 0 |
| ATOM | 918 | N | MET | B2003 | 35.809 | -1.560 | 20.439 | 1.00 33.64 | N |
| ATOM | 919 | CA | MET | B2003 | 35.239 | -2.773 | 19.791 | 1.00 33.04 | С |
| ATOM | 920 | N | | B2004 | 32.938 | -3.327 | 19.264 | 1.00 29.22 | N |
| ATOM | 921 | CA | ILE | B2004 | 31.537 | -3.604 | 19.538 | 1.00 26.95 | C |
| ATOM | 922 | CB | ILE | B2004 | 30.694 | -3.586 | 18.236 | 1.00 27.19 | С |
| ATOM | 923 | CG2 | ILE | B2004 | 29.273 | -4.070 | 18.528 | 1.00 26.67 | C |
| ATOM | 924 | CG1 | ILE | B2004 | 30.692 | -2.175 | 17.642 | 1.00 27.75 | С |
| ATOM | 925 | CD1 | ILE | B2004 | 29.965 | -2.048 | 16.307 | 1.00 28.82 | С |
| ATOM | 926 | C | ILE | B2004 | 31.452 | -4.986 | 20.165 | 1.00 25.64 | С |
| ATOM | 927 | 0 | ILE | B2004 | 32.092 | -5.924 | 19.693 | 1.00 26.78 | 0 |
| ATOM | 928 | N | | B2005 | 30.681 | -5.114 | 21.240 | 1.00 23.42 | N |
| ATOM | 929 | CA | VAL | B2005 | 30.534 | -6.406 | 21.904 | 1.00 22.67 | С |
| MOTA | 930 | CB | | B2005 | 31.099 | -6.379 | 23.344 | 1.00 23.16 | С |
| ATOM | 931 | | | B2005 | 32.615 | -6.311 | 23.305 | 1.00 22.80 | С |
| MOTA | 932 | | | B2005 | 30.552 | -5.197 | 24.096 | 1.00 23.38 | С |
| ATOM | 933 | С | VAL | B2005 | 29.086 | -6.878 | 21.948 | 1.00 21.18 | С |
| | | | | | | | | | |

| ATOM | 934 | 0 | VAL | B2005 | 28.772 | -7.884 | 22.577 | 1.00 23.33 | 0 |
|--------------|------------|-----|-----|----------------|----------------|------------------|------------------|--------------------------|--------|
| ATOM | 935 | N | | B2006 | 28.200 | -6.155 | 21.275 | 1.00 19.21 | N |
| ATOM | 936 | CA | | B2006 | 26.811 | -6.568 | 21.260 | 1.00 17.80 | С |
| MOTA | 937 | С | GLY | B2006 | 25.896 | -5.584 | 20.567 | 1.00 17.03 | С |
| ATOM | 938 | Ō | | B2006 | 26.161 | -4.387 | 20.553 | 1.00 16.68 | Ō |
| ATOM | 939 | N | | B2007 | 24.813 | -6.093 | 19.989 | 1.00 16.35 | N |
| ATOM | 940 | CA | | B2007 | 23.846 | -5.237 | 19.323 | 1.00 16.88 | C |
| ATOM | 941 | СВ | | B2007 | 24.216 | -5.042 | 17.847 | 1.00 17.35 | Ċ |
| ATOM | 942 | CG | | B2007 | 23.254 | -4.170 | 17.097 | 1.00 18.35 | c |
| ATOM | 943 | | | B2007 | 22.786 | -4.239 | 15.827 | 1.00 17.84 | Ċ |
| ATOM | 944 | | | B2007 | 22.668 | -3.058 | 17.660 | 1.00 18.04 | N |
| ATOM | 945 | | | B2007 | 21.880 | -2.479 | 16.769 | 1.00 19.69 | C |
| ATOM | 946 | | | B2007 | 21.934 | -3.176 | 15.648 | 1.00 16.84 | N |
| ATOM | 947 | С | | B2007 | 22.447 | -5.831 | 19.444 | 1.00 17.26 | C |
| ATOM | 948 | 0 | | B2007 | 22.238 | -7.027 | 19.213 | 1.00 14.74 | 0 |
| ATOM | 949 | N | | B2008 | 21.490 | -4.990 | 19.819 | 1.00 16.95 | N |
| ATOM | 950 | CA | | B2008 | 20.129 | -5.464 | 19.962 | 1.00 17.68 | C |
| ATOM | 951 | С | | B2008 | 19.095 | -4.401 | 19.661 | 1.00 18.32 | С |
| ATOM | 952 | 0 | | B2008 | 19.321 | -3.212 | 19.901 | 1.00 19.75 | 0 |
| ATOM | 953 | N | | B2009 | 17.964 | -4.830 | 19.112 | 1.00 17.31 | N |
| ATOM | 954 | CA | | B2009 | 16.868 | -3.917 | 18.821 | 1.00 18.07 | С |
| MOTA | 955 | СВ | ILE | B2009 | 16.727 | -3.598 | 17.306 | 1.00 16.33 | С |
| ATOM | 956 | CG2 | ILE | B2009 | 18.025 | -2.990 | 16.777 | 1.00 16.15 | С |
| ATOM | 957 | CG1 | ILE | B2009 | 16.361 | -4.856 | 16.519 | 1.00 19.06 | С |
| ATOM | 958 | CD1 | ILE | B2009 | 16.014 | -4.559 | 15.060 | 1.00 16.01 | С |
| ATOM | 959 | С | | B2009 | 15.607 | -4.607 | 19.312 | 1.00 17.52 | С |
| MOTA | 960 | 0 | ILE | B2009 | 15.576 | -5.827 | 19.448 | 1.00 17.73 | 0 |
| ATOM | 961 | N | ASP | B2010 | 14.580 | -3.825 | 19.607 | 1.00 18.54 | N |
| MOTA | 962 | CA | ASP | B2010 | 13.327 | -4.384 | 20.089 | 1.00 20.76 | C |
| MOTA | 963 | CB | ASP | B2010 | 13.401 | -4.663 | 21.598 | 1.00 21.38 | С |
| MOTA | 964 | CG | ASP | B2010 | 12.157 | -5.372 | 22.127 | 1.00 22.62 | С |
| MOTA | 965 | OD1 | ASP | B2010 | 11.403 | -4.762 | 22.915 | 1.00 22.62 | 0 |
| MOTA | 966 | OD2 | ASP | B2010 | 11.932 | -6.544 | 21.756 | 1.00 23.17 | 0 |
| MOTA | 967 | С | ASP | B2010 | 12.198 | -3.416 | 19.814 | 1.00 21.83 | С |
| ATOM | 968 | 0 | | B2010 | 12.378 | -2.200 | 19.912 | 1.00 21.02 | 0 |
| ATOM | 969 | N | | B2011 | 11.039 | -3.966 | 19.464 | 1.00 21.90 | N |
| ATOM | 970 | CA | | B2011 | 9.848 | -3.163 | 19.189 | 1.00 25.52 | С |
| ATOM | 971 | CB | | B2011 | 9.346 | -3.346 | 17.752 | 1.00 27.88 | С |
| ATOM | 972 | | | B2011 | 8.410 | -2.194 | 17.388 | 1.00 30.28 | C |
| ATOM | 973 | | | B2011 | 10.518 | -3.410 | 16.783 | 1.00 29.66 | C |
| ATOM | 974 | | | B2011 | 10.131 | -3.937 | 15.420 | 1.00 31.53 | C |
| ATOM | 975 | С | | B2011 | 8.738 | -3.670 | 20.102 | 1.00 24.08 | C |
| ATOM | 976 | 0 | | B2011 | 8.561 | -4.874 | 20.258 | 1.00 22.40 | 0 |
| ATOM | 977 | N | | B2012 | 8.002 | -2.757 | 20.718 | 1.00 24.39 | N |
| ATOM | 978 | CA | | B2012 | 6.911 | -3.156 | 21.598 | 1.00 24.77 | C |
| ATOM | 979 | CB | | B2012 | 7.269 | -2.868 | 23.056 | 1.00 25.42 | C |
| ATOM | 980 | CG | | B2012 | 8.482 | -3.637 | 23.554 | 1.00 28.89 | C |
| ATOM | 981 982 | CD | | B2012 B2012 | 8.233 | -5:139 | 23.652 23.721 | 1.00 31.05 | C 0 |
| ATOM ATOM | 983 | | | B2012 | 9.224 7.053 | -5.895 -5.560 | 23.721 | 1.00 31.07 1.00 30.63 | 0 |
| ATOM | 984 | C | | B2012 B2012 | 5.655 | -5.560 -2.387 | 21.208 | 1.00 30.63 | C |
| ATOM | 985 | 0 | | B2012 | 5.732 | -1.235 | 20.786 | 1.00 24.25 | 0 |
| ATOM | 986 | N | | B2012 | 4.507 | -3.043 | 21.328 | 1.00 24.45 | ท |
| ATOM | 987 | CA | | B2013 | 3.223 | -2.431 | 21.008 | 1.00 22.00 | C |
| ATOM | 988 | CB | | B2013 | 2.241 | -3.508 | 20.545 | 1.00 21.01 | C |
| ATOM | 989 | CG | | B2013 | 0.857 | -3.010 | 20.179 | 0.05 20.80 | |
| ATOM | 990 | CD | | B2013 | -0.106 | -4.152 | 19.921 | 0.05 20.56 | Č |
| | | | | | _ | _ | | | |

| ATOM | 991 | OE1 | GLU | B2013 | 0.231 | -5.039 | 19.109 | 0.05 20.26 | 0 |
|--------------|--------------|---------|-----|----------------|------------------|--------------------|------------------|--------------------------|--------|
| ATOM | 992 | OE2 | GLU | B2013 | -1.196 | -4.166 | 20.529 | 0.05 20.00 | 0 |
| MOTA | 993 | С | GLU | B2013 | 2.719 | -1.793 | 22.292 | 1.00 20.42 | , C |
| ATOM | 994 | 0 | GLU | B2013 | 2.644 | -2.457 | .23.326 | 1.00 19.82 | 0 |
| ATOM | 995 | N | LEU | B2014 | 2.383 | -0.512 | 22.244 | 1.00 20.95 | N |
| MOTA | 996 | CA | LEU | B2014 | 1.906 | 0.149 | 23.452 | 1.00 25.05 | С |
| MOTA | 997 | CB | LEU | B2014 | 1.530 | 1.604 | 23.162 | 1.00 26.46 | C |
| MOTA | 998 | CG | | B2014 | 2.610 | 2.478 | 22.521 | 1.00 29.15 | С |
| ATOM | 999 | CD1 | LEU | B2014 | 2.171 | 3. 9 29 | 22.610 | 1.00 32.28 | С |
| ATOM | 1000 | CD2 | LEU | B2014 | 3.945 | 2.294 | 23.225 | 1.00 28.39 | С |
| MOTA | 1001 | С | LEU | B2014 | 0.708 | -0.582 | 24.053 | 1.00 25.52 | C |
| MOTA | 1002 | 0 | LEU | B2014 | 0.635 | -0.773 | 25.266 | 1.00 25.48 | 0 |
| MOTA | 1003 | N | ALA | B2015 | -0.220 | -1.001 | 23.196 | 1.00 26.92 | N |
| MOTA | 1004 | CA | ALA | B2015 | -1.425 | -1.697 | 23.637 | 1.00 28.21 | С |
| MOTA | 1005 | CB | ALA | B2015 | -2.267 | -2.088 | 22.426 | 1.00 29.71 | C |
| MOTA | 1006 | С | ALA | B2015 | -1.144 | -2.932 | 24.490 | 1.00 29.10 | C |
| ATOM | 1007 | 0 | | B2015 | -1.864 | -3.208 | 25.450 | 1.00 29.79 | 0 |
| MOTA | 1008 | N | SER | B2016 | -0.106 | -3.681 | 24.135 | 1.00 29.36 | N |
| ATOM | 1009 | CA | | B2016 | 0.246 | -4.885 | 24.875 | 1.00 30.31 | C |
| MOTA | 1010 | CB | SER | B2016 | 1.357 | -5.633 | 24.147 | 1.00 32.28 | C |
| MOTA | 1011 | OG | | B2016 | 1.032 | -5.782 | 22.779 | 1.00 33.64 | 0 |
| ATOM | 1012 | С | | B2016 | 0.705 | -4.508 | 26.275 | 1.00 30.37 | С |
| ATOM | 1013 | 0 | | B2016 | 0.369 | -5.170 | 27.260 | 1.00 29.37 | 0 |
| MOTA | 1014 | N | | B2017 | 1.476 | -3.431 | 26.353 | 1.00 30.04 | N |
| ATOM | 1015 | CA | ILE | B2017 | 1.979 | -2.955 | 27.625 | 1.00 30.17 | С |
| ATOM | 1016 | CB | | B2017 | 2.907 | -1.741 | 27.420 | 1.00 29.67 | C |
| ATOM | 1017 | CG2 | ILE | B2017 | 3.323 | -1.153 | 28.765 | 1.00 31.54 | С |
| ATOM | 1018 | | | B2017 | 4.141 | -2.178 | 26.630 | 1.00 29.63 | С |
| MOTA | 1019 | | | B2017 | 4.883 | -3.368 | 27.246 | 1.00 29.53 | С |
| ATOM | 1020 | С | | B2017 | 0.814 | -2.585 | 28.537 | 1.00 30.53 | С |
| ATOM | 1021 | 0 | | B2017 | 0.736 | -3.051 | 29.673 | 1.00 29.90 | 0 |
| ATOM | 1022 | N | | B2018 | -0.100 | -1.762 | 28.03,4 | 1.00 31.91 | N |
| ATOM | 1023 | CA | | B2018 | -1.252 | -1.363 | 28.831 | 1.00 34.92 | C |
| MOTA | 1024 | CB | | B2018 | -2.113 | -0.355 | 28.064 | 1.00 37.97 | С |
| ATOM | 1025 | CG | | B2018 | -1.895 | -0.370 | 26.565 | 1.00 42.86 | C |
| MOTA | 1026 | CD | | B2018 | -2.698 | 0.700 | 25.844 | 1.00 45.97 | C |
| ATOM | 1027 | | | B2018 | -3.945 | 0.608 | 25.843 | 1.00 47.86 | 0 |
| ATOM | 1028 | | | B2018 | -2.084 | 1.633 | 25.279 | 1.00 47.02 | 0 |
| ATOM | 1029 | C | | B2018 | -2.085 | -2.573 | 29.247 | 1.00 34.56 | C |
| MOTA | 1030 | 0 | | B2018 | -2.490 | -2.678 | 30.404 | 1.00 35.89 | 0 |
| ATOM ATOM | 1031 1032 | N CA | | B2019 B2019 | -2.349 | -3.488 | 28.321 | 1.00 33.29 | N |
| ATOM | 1032 | CB | | B2019 | -3.117 -3.270 | -4.674 -5.623 | 28.681 27.490 | 1.00 33.75 1.00 32.73 | C C |
| ATOM | 1033 | OG | | B2019 | -4.314 | -5.203 | 26.635 | 1.00 32.73 | 0 |
| ATOM | 1035 | C | | B2019 | -2.416 | | 29.822 | | c |
| ATOM | 1036 | Ö | | B2019 | -3.066 | -5.963 | 30.698 | 1.00 33.12 | 0 |
| ATOM | 1037 | N | | B2020 | -1.087 | ÷5.398 | 29.808 | 1.00 32.03 | И |
| ATOM | 1038 | CA | | B2020 | -0.329 | -6:055 | 30.869 | 1.00 35.22 | C |
| ATOM | 1039 | CB | | B2020 | 1.157 | -6.105 | 30.510 | 1.00 33.30 | c |
| ATOM | 1040 | C | | B2020 | -0.537 | -5.295 | 32.179 | 1.00 34.07 | c |
| ATOM | 1041 | Ö | | B2020 | -0.669 | -5.898 | 33.241 | 1.00 30.00 | 0 |
| ATOM | 1042 | N | | B2021 | -0.570 | -3.968 | 32.097 | 1.00 34.70 | N |
| ATOM | 1043 | CA | | B2021 | -0.783 | -3.133 | 33.277 | 1.00 42.15 | C |
| ATOM | 1044 | CB | | B2021 | -0.672 | -1.627 | 32.931 | 1.00 42.05 | C |
| ATOM | 1045 | | | B2021 | -1.060 | -0.775 | 34.138 | 1.00 42.48 | c |
| ATOM | 1046 | | | B2021 | 0.746 | -1.298 | 32.504 | 1.00 42.42 | C |
| MOTA | 1047 | С | | B2021 | -2.176 | -3.410 | 33.841 | 1.00 44.98 | Ċ |

| ATOM | 1048 | 0 | VAT. | B2021 | -2.491 | -3.029 | 34.967 | 1.00 45.67 | 0 |
|------|------|-----|------|-------|--------|---------|--------|------------|-----|
| ATOM | 1049 | N | | B2022 | -3.001 | -4.085 | 33.047 | 1.00 47.50 | N |
| ATOM | 1050 | CA | | B2022 | -4.359 | -4.420 | 33.451 | 1.00 47.30 | C |
| ATOM | 1051 | CB | | B2022 | -5.323 | -4.368 | | | |
| | | | | | | | 32.236 | 1.00 51.16 | С |
| ATOM | 1052 | | | B2022 | -5.501 | -3.007 | 31.824 | 1.00 53.24 | 0 |
| ATOM | 1053 | | | B2022 | -6.677 | -4.957 | 32.592 | 1.00 52.95 | С |
| ATOM | 1054 | С | | B2022 | -4.454 | -5.799 | 34.109 | 1.00 50.81 | C |
| ATOM | 1055 | 0 | THR | B2022 | -4.937 | -5.918 | 35.232 | 1.00 51.36 | 0 |
| MOTA | 1056 | N | ARG | B2023 | -3.988 | -6.836 | 33.421 | 1.00 51.25 | N |
| ATOM | 1057 | CA | ARG | B2023 | -4.064 | -8.187 | 33.968 | 1.00 52.22 | С |
| ATOM | 1058 | CB | ARG | B2023 | -3.746 | -9.220 | 32.883 | 1.00 52.29 | С |
| ATOM | 1059 | CG | ARG | B2023 | -4.157 | -10.644 | 33.242 | 0.05 51.97 | С |
| ATOM | 1060 | CD | | B2023 | | -10.663 | 33.905 | 0.05 51.83 | c |
| ATOM | 1061 | NE | | B2023 | | -11.966 | 33.828 | 0.05 51.66 | N |
| ATOM | 1062 | CZ | | B2023 | | -12.474 | 32.713 | 0.05 51.57 | C |
| ATOM | 1063 | | | B2023 | | -11.789 | 31.579 | 0.05 51.47 | N |
| ATOM | 1064 | | | B2023 | | | | | |
| | | | | | | -13.663 | 32.730 | 0.05 51.49 | N |
| MOTA | 1065 | C | | B2023 | -3.157 | | 35.173 | 1.00 53.22 | C |
| ATOM | 1066 | 0 | | B2023 | -3.256 | -9.424 | 35.859 | 1.00 53.07 | 0 |
| ATOM | 1067 | N | | B2024 | -2.274 | -7.447 | 35.432 | 1.00 53.34 | N |
| MOTA | 1068 | CA | | B2024 | -1.365 | -7.544 | 36.564 | 1.00 53.62 | С |
| MOTA | 1069 | CB | HIS | B2024 | -0.042 | -8.176 | 36.127 | 1.00 54.97 | C |
| ATOM | 1070 | CG | HIS | B2024 | -0.208 | -9.477 | 35.403 | 1.00 56.91 | С |
| ATOM | 1071 | CD2 | HIS | B2024 | -0.006 | -10.755 | 35.805 | 1.00 57.80 | С |
| ATOM | 1072 | ND1 | HIS | B2024 | -0.660 | -9.552 | 34.103 | 1.00 57.75 | N |
| MOTA | 1073 | CE1 | HIS | B2024 | | -10.820 | 33.735 | 1.00 58.06 | С |
| ATOM | 1074 | | | B2024 | | -11.570 | 34.750 | 1.00 57.59 | N |
| ATOM | 1075 | С | | B2024 | -1.127 | | 37.148 | 1.00 53.35 | . C |
| ATOM | 1076 | Ö | | B2024 | -0.312 | | 36.644 | 1.00 53.29 | . 0 |
| ATOM | 1077 | N | | B2025 | -1.861 | | 38.214 | 1.00 52.80 | N N |
| ATOM | 1078 | CA | • | B2025 | -1.785 | -4.569 | 38.905 | 1.00 52.80 | C |
| ATOM | 1079 | | | | | | | | |
| | | CB | | B2025 | -2.618 | -4.637 | 40.188 | 1.00 54.49 | C |
| ATOM | 1080 | CG | | B2025 | -4.095 | -4.920 | 39.949 | 1.00 56.85 | C |
| ATOM | 1081 | CD | | B2025 | -4.798 | -5.434 | 41.190 | 1.00 58.84 | C |
| ATOM | 1082 | | | B2025 | -4.520 | -6.584 | 41.595 | 1.00 60.08 | 0 |
| ATOM | 1083 | | | B2025 | -5.624 | -4.690 | 41.763 | 1.00 59.42 | 0 |
| ATOM | 1084 | С | | B2025 | -0.364 | -4.122 | 39.247 | 1.00 48.83 | С |
| MOTA | 1085 | 0 | GLU | B2025 | -0.058 | -2.931 | 39.211 | 1.00 48.34 | 0 |
| MOTA | 1086 | N | GLY | B2026 | 0.497 | -5.074 | 39.588 | 1.00 45.49 | N |
| ATOM | 1087 | CA | GLY | B2026 | 1.864 | -4.729 | 39.932 | 1.00 40.95 | С |
| ATOM | 1088 | С | GLY | B2026 | 2.826 | -4.920 | 38.774 | 1.00 37.63 | C |
| MOTA | 1089 | 0 - | GLY | B2026 | 4.027 | -5.077 | 38.978 | 1.00 37.06 | 0 |
| MOTA | 1090 | N | PHE | B2027 | 2.301 | -4.902 | 37.554 | 1.00 33.22 | N |
| MOTA | 1091 | CA | PHE | B2027 | 3.135 | -5.083 | 36.374 | 1.00 30.35 | С |
| ATOM | 1092 | СВ | PHE | B2027 | 2.287 | -4.995 | 35.105 | 1.00 29.47 | С |
| MOTA | 1093 | CG | | B2027 | 3.079 | | 33.840 | 1.00 28.37 | C |
| ATOM | 1094 | | | B2027 | 3.501 | | 33.431 | 1.00 28.75 | Ċ |
| ATOM | 1095 | | | B2027 | 3.432 | | 33.076 | 1.00 26.82 | Ċ |
| ATOM | 1096 | | | B2027 | 4.264 | -6.575 | 32.277 | 1.00 27.85 | Č |
| ATOM | 1097 | | | B2027 | 4.195 | | 31.919 | 1.00 27.50 | C |
| ATOM | 1097 | CZ | | B2027 | 4.611 | | 31.520 | 1.00 27.30 | c |
| ATOM | | | | | | | | 1.00 28.11 | |
| | 1099 | C | | B2027 | 4.245 | | 36.303 | | C |
| ATOM | 1100 | 0 | | B2027 | 5.419 | | 36.179 | 1.00 27.55 | 0 |
| ATOM | 1101 | N | | B2028 | 3.863 | | 36.376 | 1.00 26.54 | N |
| ATOM | 1102 | CA | | B2028 | 4.820 | | 36.306 | 1.00 26.97 | C |
| ATOM | 1103 | CB | | B2028 | 4.103 | | 36.503 | 1.00 26.06 | C |
| ATOM | 1104 | С | ALA | B2028 | 5.938 | -1.815 | 37.329 | 1.00 27.20 | С |
| | | | | | | | | | |

| ATOM | 1105 | 0 | ALA | B2028 | 7.112 | -1.697 | 36.998 | 1.00 26.33 | 0 |
|--------------|--------------|-----------|-----|----------------|------------------|----------------|------------------|--------------------------|--------|
| ATOM | 1106 | N | LYS | B2029 | 5.555 | -2.075 | 38.572 | 1.00 28.14 | N |
| MOTA | 1107 | CA | LYS | B2029 | 6.496 | -2.213 | 39.673 | 1.00 30.24 | С |
| MOTA | 1108 | CB | LYS | B2029 | 5.738 | -2.543 | 40.965 | 1.00 33.94 | С |
| MOTA | 1109 | CG | LYS | B2029 | 6.597 | -2.502 | 42.215 | 1.00 39.10 | С |
| MOTA | 1110 | CD | LYS | B2029 | 7.038 | -1.082 | 42.540 | 1.00 42.39 | С |
| MOTA | 1111 | CE | | B2029 | 8.108 | -1.070 | 43.629 | 1.00 45.14 | C |
| MOTA | 1112 | NZ | LYS | B2029 | 7.712 | -1.858 | 44.836 | 1.00 46.16 | N |
| ATOM | 1113 | С | LYS | B2029 | 7.567 | -3.264 | 39.437 | 1.00 28.56 | С |
| ATOM | 1114 | 0 | | B2029 | 8.696 | -3.114 | 39.902 | 1.00 28.42 | 0 |
| MOTA | 1115 | N | | B2030 | 7.219 | -4.325 | 38.717 | 1.00 26.96 | N |
| ATOM | 1116 | CA | ARG | B2030 | 8.171 | -5.397 | 38.452 | 1.00 25.76 | С |
| ATOM | 1117 | CB | ARG | B2030 | 7.430 | -6.708 | 38.180 | 1.00 27.87 | С |
| MOTA | 1118 | CG | | B2030 | 6.318 | -7.007 | 39.174 | 0.05 26.73 | С |
| MOTA | 1119 | CD | | B2030 | 6.358 | -8.451 | 39.652 | 0.05 26.68 | С |
| ATOM | 1120 | NE | ARG | B2030 | 6.295 | -9.416 | 38.557 | 0.05 26.45 | N |
| ATOM | 1121 | CZ | ARG | B2030 | 5.263 | -9.553 | 37.730 | 0.05 26.36 | С |
| MOTA | 1122 | | | B2030 | 4.191 | -8.783 | 37.862 | 0.05 26.22 | N |
| MOTA | 1123 | NH2 | ARG | B2030 | | -10.469 | 36.771 | 0.05 26.29 | N |
| MOTA | 1124 | Ç | | B2030 | 9.069 | -5.076 | 37.266 | 1.00 24.16 | С |
| MOTA | 1125 | 0 | | B2030 | 10.200 | -5.551 | 37.187 | 1.00 22.83 | 0 |
| MOTA | 1126 | N | | B2031 | 8.559 | -4.270 | 36.341 | 1.00 22.75 | N |
| ATOM | 1127 | CA | | B2031 | 9.319 | -3.903 | 35.158 | 1.00 22.54 | С |
| ATOM | 1128 | CB | | B2031 | 8.371 | -3.536 | 33.984 | 1.00 23.94 | С |
| MOTA | 1129 | | | B2031 | 9.156 | -2.884 | 32.855 | 1.00 24.54 | С |
| MOTA | 1130 | | | B2031 | 7.677 | -4.794 | 33.467 | 1.00 24.38 | С |
| MOTA | 1131 | С | | B2031 | 10.264 | -2.739 | 35.409 | 1.00 21.20 | С |
| MOTA | 1132 | 0 | | B2031 | 11.364 | -2.699 | 34.858 | 1.00 21.89 | 0 |
| MOTA | 1133 | N | | B2032 | 9.837 | -1.805 | 36.252 | 1.00 20.43 | N |
| ATOM | 1134 | CA | | B2032 | 10.623 | -0.607 | 36.552 | 1.00 21.46 | С |
| ATOM | 1135 | CB | | B2032 | 9.722 | 0.624 | 36.459 | 1.00 21.16 | C |
| ATOM | 1136 | CG | | B2032 | | 0.814 | 35.180 | 1.00 22.44 | С |
| ATOM | 1137 | | | B2032 | 7.913 | 1.951 | 35.383 | 1.00 25.05 | C |
| ATOM | 1138 | | | B2032 | 9.822 | 1.107 | 34.003 | 1.00 23.51 | C |
| ATOM | 1139 | C | | B2032 | 11.289 | -0.613 | 37.928 | 1.00 20.88 | C |
| ATOM | 1140 | 0 | | B2032 B2033 | 10.758 | -1.188 | 38.875 | 1.00 24.06 | 0 |
| ATOM ATOM | 1141 | N CA | | B2033 | 12.451 13.147 | 0.027 0.117 | 38.035 39.317 | 1.00 20.86 1.00 20.81 | N C |
| ATOM | 1142 | CA | | B2033 | 14.602 | 0.569 | 39.160 | 1.00 20.81 | C |
| ATOM | 1143 1144 | CB OG1 | | B2033 | 14.623 | 1.853 | 38.521 | 1.00 20.39 | 0 |
| ATOM | 1145 | | | B2033 | 15.394 | -0.443 | 38.341 | 1.00 21.21 | C |
| ATOM | 1145 | C | | B2033 | 12.432 | 1.189 | 40.119 | 1.00 20.37 | C |
| ATOM | 1147 | 0 | | B2033 | 11.479 | 1.806 | 39.635 | 1.00 21.74 | 0 |
| ATOM | 1148 | N | | B2034 | 12.893 | 1.427 | 41.339 | 1.00 22.64 | N |
| ATOM | 1149 | CA | | B2034 | 12.267 | 2.441 | 42.177 | 1.00 24.18 | c |
| ATOM | 1150 | СВ | | B2034 | 12.939 | 2.479 | 43.541 | 1.00 24.55 | C |
| ATOM | 1151 | C | | B2034 | 12.371 | 3.806 | 41.502 | 1.00 25.08 | c |
| ATOM | 1152 | Ō | | B2034 | 11.393 | 4.555 | 41.437 | 1.00 24.57 | Ō |
| ATOM | 1153 | N | | B2035 | 13.558 | 4.119 | 40.989 | 1.00 25.67 | N |
| ATOM | 1154 | CA | | B2035 | 13.786 | 5.403 | 40.337 | 1.00 27.37 | C |
| ATOM | 1155 | CB | | B2035 | 15.274 | 5.576 | 40.025 | 1.00 30.75 | C |
| ATOM | 1156 | CG | | B2035 | 15.792 | 7.017 | 40.016 | 1.00 34.25 | Č |
| ATOM | 1157 | | | B2035 | 15.529 | 7.681 | 41.373 | 1.00 34.25 | Č |
| ATOM | 1158 | | | B2035 | 17.286 | 7.010 | 39.715 | 1.00 36.03 | C |
| ATOM | 1159 | C | | B2035 | 12.948 | 5.550 | 39.066 | 1.00 26.19 | Ċ |
| ATOM | 1160 | ō | | B2035 | 12.424 | 6.625 | 38.789 | 1.00 25.81 | 0 |
| ATOM | 1161 | N | | B2036 | 12.829 | 4.479 | 38.288 | 1.00 24.86 | N |
| | | | | | | | | | |

| ATOM | 1162 | CA | GLU | B2036 | 12.010 | 4.523 | 37.074 | 1.00 24.94 | С |
|------|------|------|-----|---------|--------|----------------|------------------|------------|--------|
| MOTA | 1163 | CB | GLU | B2036 | 12.218 | 3.256 | 36.238 | 1.00 24.20 | С |
| MOTA | 1164 | CG | GLU | B2036 | 13.521 | 3.220 | 35.439 | 1.00 22.34 | С |
| MOTA | 1165 | CD · | GLU | B2036 | 13.823 | 1.834 | 34.878 | 1.00 22.43 | С |
| ATOM | 1166 | OE1 | GLU | B2036 | 14.592 | 1.744 | 33.899 | 1.00 20.15 | 0 |
| MOTA | 1167 | OE2 | GLU | B2036 | 13.302 | 0.834 | 35.425 | 1.00 21.31 | 0 |
| ATOM | 1168 | С | GLU | B2036 | 10.528 | 4.645 | 37.461 | 1.00 25.14 | С |
| ATOM | 1169 | O | | B2036 | 9.740 | 5.261 | 36.746 | 1.00 24.49 | 0 |
| ATOM | 1170 | | | B2037 | 10.155 | 4.051 | 38.593 | 1.00 25.36 | N |
| ATOM | 1171 | CA | | B2037 | 8.772 | 4.116 | 39.067 | 1.00 27.03 | С |
| ATOM | 1172 | СВ | | B2037 | 8.570 | 3.202 | 40.279 | 1.00 28.19 | С |
| ATOM | 1173 | | | B2037 | 8.077 | 1.811 | 39.932 | 1.00 30.50 | С |
| ATOM | 1174 | SD | | B2037 | 6.592 | 1.878 | 38.903 | 1.00 35.36 | S |
| ATOM | 1175 | CE | | B2037 | 5.315 | 2.130 | 40.111 | 1.00 31.11 | С |
| ATOM | 1176 | C | | B2037 | 8.389 | 5.541 | 39.445 | 1.00 27.51 | С |
| ATOM | 1177 | ŏ | | B2037 | 7.288 | 6.004 | 39.146 | 1.00 27.72 | 0 |
| ATOM | 1178 | N | | B2038 | 9.309 | 6.232 | 40.104 | 1.00 29.26 | N |
| ATOM | 1179 | CA | | B2038 | 9.075 | 7.604 | 40.522 | 1.00 30.50 | C |
| | 1180 | CB | | B2038 | 10.261 | 8.089 | 41.363 | 1.00 33.66 | С |
| ATOM | | CG | | B2038 | 10.100 | 7.747 | 42.852 | 1.00 38.27 | С |
| ATOM | 1181 | CD | | B2038 | 11.384 | 7.278 | 43.517 | 1.00 41.20 | C |
| ATOM | 1182 | | | B2038 | 12.448 | 7.886 | 43.264 | 1.00 41.95 | Ō |
| ATOM | 1183 | | | B2038 | 11.322 | 6.307 | 44.309 | 1.00 42.56 | ő |
| ATOM | 1184 | | | | | 8.512 | 39.320 | 1.00 29.98 | Ċ |
| ATOM | 1185 | C | | B2038 | 8.827 | 9.473 | 39.403 | 1.00 29.40 | ō |
| ATOM | 1186 | 0 | | B2038 | 8.059 | 8.198 | 38.198 | 1.00 28.37 | N |
| ATOM | 1187 | N | | B2039 | 9.465 | 8.973 | 36.986 | 1.00 28.60 | c |
| ATOM | 1188 | CA | | B2039 | 9.272 | | 35.973 | 1.00 32.59 | c |
| ATOM | 1189 | CB | | B2039 | 10.374 | 8.670 | | 1.00 36.59 | č |
| ATOM | 1190 | CG | | B2039 | 10.103 | 9.236 | 34.589 34.627 | 1.00 42.20 | č |
| ATOM | 1191 | CD | | B2039 | 9.892 | 10.740 | 33.284 | 1.00 42.20 | Ŋ |
| MOTA | 1192 | NE | | B2039 | 9.750 | 11.301 | | 1.00 48.88 | C |
| MOTA | 1193 | CZ | | B2039 | 9.599 | 12.597 | 33.025 31.770 | 1.00 48.84 | Ŋ |
| MOTA | 1194 | | | B2039 | 9.477 | 13.014 | 34.018 | 1.00 49.51 | N |
| ATOM | 1195 | | | B2039 | 9.570 | 13.478 | | 1.00 49.31 | C |
| ATOM | 1196 | С | | B2039 | 7.926 | 8.585 | 36.397 | 1.00 27.40 | ő |
| MOTA | 1197 | 0 | | B2039 | 7.107 | 9.439 | 36.047 36.291 | 1.00 25.73 | N |
| MOTA | 1198 | N | | B2040 | 7.717 | 7.280 | | 1.00 25.75 | C |
| MOTA | 1199 | CA | | B2040 | 6.489 | 6.710 | 35.758 | 1.00 20.22 | c |
| ATOM | 1200 | СВ | | B2040 | 6.546 | 5.185 | 35.916 | 1.00 24.51 | Č |
| MOTA | 1201 | CG | | B2040 | 5.265 | 4.477 | 35.573 34.248 | 1.00 26.83 | Ċ |
| ATOM | 1202 | | | B2040 | 4.871 | 4.318 3.938 | 36.579 | 1.00 26.24 | c |
| ATOM | 1203 | | | B2040 | 4.467 | | 33.930 | 1.00 27.58 | c |
| ATOM | 1204 | | | B2040 | 3.698 | 3.627 | 36.276 | 1.00 27.33 | Č |
| MOTA | 1205 | | | B2040 | 3.297 | 3.249 | 34.950 | 1.00 27.41 | Č |
| MOTA | 1206 | CZ | | B2040 | 2.911 | 3.090 | | 1.00 27.03 | č |
| MOTA | 1207 | С | | B2040 | 5.245 | 7.262 | 36.463 | 1.00 20.33 | ő |
| ATOM | 1208 | 0 | | B2040 | 4.269 | - 7.622 | 35.814 | 1.00 27.19 | N |
| MOTA | 1209 | N | | B2041 | 5.287 | 7:324 | 37.792 38.575 | 1.00 27.13 | C |
| ATOM | 1210 | CA | | B2041 | 4.151 | 7.805 | | 1.00 27.42 | Č |
| MOTA | 1211 | CB | | B2041 | 4.328 | 7.485 | 40.078 | | ō |
| ATOM | 1212 | | | B2041 | 5.504 | 8.132 | 40.577 | 1.00 28.52 | c |
| ATOM | 1213 | | | B2041 | 4.458 | 5.986 | 40.294 | 1.00 28.04 | C |
| MOTA | 1214 | С | | B2041 | 3.896 | 9.304 | 38.432 | 1.00 28.31 | |
| ATOM | 1215 | 0 | | R B2041 | 2.840 | 9.796 | 38.840 | | O N |
| ATOM | 1216 | N | | R B2042 | 4.854 | 10.024 | 37.853 | | И С |
| MOTA | 1217 | CA | | R B2042 | 4.706 | 11.465 | 37.665 | | · C |
| MOTA | 1218 | СВ | SEF | R B2042 | 6.039 | 12.179 | 37.896 | 1.00 32.90 | C |
| | | | | | | | | | |

| MOTA | 1219 | OG | SER | B2042 | 6.326 | 12.278 | 39.282 | 1.00 36.54 | 0 |
|--------------|--------------|----|------|----------------|----------------|--------|--------|------------|-----|
| MOTA | 1220 | | | B2042 | 4.168 | 11.841 | 36.289 | 1.00 31.32 | С |
| ATOM | 1221 | | SER | B2.042 | 3.909 | 13.012 | 36.018 | 1.00 30.89 | 0 |
| ATOM | 1222 | | | B2043 | 4.008 | 10.849 | 35.421 | 1.00 31.83 | N |
| MOTA | 1223 | | LEU | B2043 | 3.487 | 11.088 | 34.077 | 1.00 31.92 | С |
| ATOM | 1224 | | | B2043 | 4.293 | 10.300 | 33.038 | 1.00 29.48 | C |
| ATOM | 1225 | | | B2043 | 5.785 | 10.603 | 32.912 | 1.00 29.62 | С |
| ATOM | 1226 | | | B2043 | 6.420 | 9.633 | 31.921 | 1.00 29.54 | С |
| ATOM | 1227 | | | B2043 | 5.985 | 12.035 | 32.462 | 1.00 29.33 | С |
| | 1228 | | | B2043 | 2.039 | 10.623 | 34.058 | 1.00 33.01 | С |
| ATOM ATOM | 1229 | | | B2013 | 1.569 | 10.030 | 35.026 | 1.00 32.48 | . 0 |
| | 1230 | _ | | B2044 | 1.337 | 10.877 | 32.957 | 1.00 36.01 | N |
| MOTA | 1231 | CA | | B2044 | -0.060 | 10.469 | 32.850 | 1.00 38.06 | С |
| ATOM | 1231 | CB | | B2044 | -0.967 | 11.586 | 33.375 | 1.00 39.86 | С |
| ATOM | 1232 | CG | | B2044 | -2.402 | 11.149 | 33.619 | 1.00 43.44 | С |
| MOTA | | CD | | B2044 | -3.295 | 12.317 | 34.013 | 1.00 45.82 | С |
| ATOM | 1234 1235 | CE | | B2044 | -4.630 | 11.825 | 34.554 | 1.00 46.21 | С |
| ATOM | | | | B2044 | -5.292 | 10.879 | 33.615 | 1.00 47.83 | N |
| MOTA | 1236 | NZ | | B2044 | -0.472 | 10.116 | 31.422 | 1.00 38.81 | С |
| ATOM | 1237 | C | | B2044 | 0.225 | 10.438 | 30.459 | 1.00 39.23 | 0 |
| ATOM | 1238 | 0 | | B2044 B2045 | -1.611 | 9.443 | 31.299 | 1.00 39.57 | N |
| MOTA | 1239 | N | - | | -2.134 | 9.068 | 29.996 | 1.00 40.10 | С |
| MOTA | 1240 | CA | - | B2045 | -1.177 | 8.355 | 29.062 | 1.00 40.74 | C |
| MOTA | 1241 | C | | B2045 | -0.513 | 7.394 | 29.454 | 1.00 41.23 | Ō |
| MOTA | 1242 | 0 | | B2045 | -1.115 | 8.832 | 27.820 | 1.00 41.17 | N |
| MOTA | 1243 | N | | B2046 | -0.255 | 8.249 | 26.791 | 1.00 41.02 | c |
| MOTA | 1244 | CA | | B2046 | -0.396 | 9.015 | 25.472 | 1.00 43.31 | C |
| ATOM | 1245 | CB | | B2046 | | 9.015 | 24.931 | 1.00 47.77 | č |
| ATOM | 1246 | CG | | B2046 | -1.812 | 9.873 | 23.627 | 1.00 50.51 | Ċ |
| ATOM | 1247 | CD | | B2046 | -1.882 | 10.180 | 23.244 | 1.00 52.23 | N |
| ATOM | 1248 | NE | | B2046 | -3.260 | 10.768 | 22.103 | 1.00 52.56 | C |
| MOTA | 1249 | CZ | | B2046 | -3.611 | 11.012 | 21.844 | 1.00 52.50 | N |
| ATOM | 1250 | | | B2046 | -4.890 | 11.107 | 21.217 | 1.00 53.75 | N |
| MOTA | 1251 | | | B2046 | -2.684 | 8.229 | 27.184 | 1.00 39.59 | C |
| ATOM | 1252 | C | | B2046 | 1.212 1.873 | 7.198 | 27.104 | 1.00 38.95 | ō |
| ATOM | 1253 | 0 | | B2046 | | 9.375 | 27.631 | 1.00 38.59 | N |
| ATOM | 1254 | N | | B2047 | 1.718 | 9.492 | 28.022 | 1.00 36.93 | C |
| MOTA | 1255 | CA | | B2047 | 3.117 | 10.914 | 28.497 | 1.00 30.53 | č |
| MOTA | 1256 | CB | | B2047 | 3.415 | 11.965 | 27.408 | 1.00 43.89 | c |
| MOTA | 1257 | CG | | B2047 | 3.284 3.915 | 13.275 | 27.843 | 1.00 46.98 | c |
| MOTA | 1258 | CD | | B2047 | 5.322 | 13.273 | 28.189 | 1.00 49.81 | N |
| ATOM | 1259 | NE | | B2047 | 6.145 | 14.072 | 28.545 | 1.00 50.90 | C |
| ATOM | 1260 | CZ | | B2047 | 5.708 | 15.324 | 28.603 | 1.00 51.65 | N |
| ATOM | 1261 | | | B2047 | 7.409 | 13.800 | 28.845 | 1.00 52.13 | N |
| ATOM | 1262 | | | B2047 | 3.543 | 8.496 | 29.095 | 1.00 34.22 | С |
| ATOM | 1263 | C | | B2047 | 4.671 | 8.017 | 29.086 | | Ō |
| MOTA | 1264 | 0 | | B2047 | 2.646 | | 30.022 | | N |
| ATOM | 1265 | N | | B2048 | 2.968 | | 31.081 | | C |
| MOTA | 1266 | | | B2048 | | | 32.121 | | Č |
| ATOM | 1267 | | | B2048 | 1.844 2.236 | | 33.420 | | c |
| MOTA | 1268 | | | N B2048 | | | 34.415 | | c |
| ATOM | 1269 | CD | | N B2048 | 1.089 | | 35.596 | | ō |
| MOTA | 1270 | | | N B2048 | 1.297 | | | | N |
| MOTA | 1271 | | | N B2048 | -0.125 | | | | C |
| ATOM | 1272 | | | N B2048 | 3.161 | | | | ō |
| ATOM | 1273 | | | N B2048 | 4.134 | | | | N |
| ATOM | 1274 | | | E B2049 | 2.230 | | | | C |
| MOTA | 1275 | CA | i Li | E B2049 | 2.318 | 7.139 | 20.701 | . 1.00 200 | _ |
| | | | | | | | | | |

| ATOM | 1276 | CB | ILE | B2049 | | 1.099 | 3.894 | 28.053 | 1.00 24.71 | C |
|------|------|-----|-----|---------|---|--------|--------|--------|------------|---|
| MOTA | 1277 | CG2 | ILE | B2049 | | 1.310 | 2.606 | 27.254 | 1.00 25.39 | С |
| ATOM | 1278 | CG1 | ILE | B2049 | | -0.174 | 3.814 | 28.906 | 1.00 25.99 | С |
| MOTA | 1279 | CD1 | ILE | B2049 | | -0.111 | 2.776 | 30.004 | 1.00 26.01 | С |
| MOTA | 1280 | С | ILE | B2049 | | 3.570 | 4.090 | 28.104 | 1.00 23.58 | С |
| ATOM | 1281 | 0 | ILE | B2049 | | 4.281 | 3.091 | 28.120 | 1.00 24.35 | 0 |
| ATOM | 1282 | N | GLU | B2050 | | 3.828 | 5.160 | 27.360 | 1.00 22.52 | N |
| ATOM | 1283 | | GLU | B2050 | | 4.985 | 5.238 | 26.482 | 1.00 23.92 | С |
| ATOM | 1284 | | | B2050 | | 4.980 | 6.575 | 25.739 | 1.00 24.81 | C |
| ATOM | 1285 | CG | | B2050 | | 6.216 | 6.842 | 24.901 | 1.00 27.69 | С |
| ATOM | 1286 | CD | | B2050 | | 6.470 | 5.767 | 23.859 | 1.00 30.29 | С |
| ATOM | 1287 | | | B2050 | | 5.514 | 5.384 | 23.149 | 1.00 32.11 | 0 |
| ATOM | 1288 | | | B2050 | | 7.632 | 5.314 | 23.740 | 1.00 29.75 | 0 |
| ATOM | 1289 | C | | B2050 | | 6.278 | 5.085 | 27.270 | 1.00 23.59 | С |
| ATOM | 1290 | 0 | | B2050 | | 7.235 | 4.452 | 26.804 | 1.00 23.37 | 0 |
| ATOM | 1291 | N | | B2051 | | 6.304 | 5.666 | 28.466 | 1.00 23.27 | N |
| ATOM | 1292 | CA | | B2051 | | 7.487 | 5.584 | 29.306 | 1.00 23.17 | С |
| ATOM | 1293 | СВ | | B2051 | | 7.300 | 6.397 | 30.592 | 1.00 22.74 | С |
| ATOM | 1294 | CG | | B2051 | | 8.520 | 6.367 | 31.492 | 1.00 22.74 | С |
| ATOM | 1295 | | | B2051 | | 8.667 | 5.382 | 32.474 | 1.00 21.76 | С |
| ATOM | 1296 | | | B2051 | | 9.818 | 5.317 | 33.263 | 1.00 23.29 | С |
| ATOM | 1297 | | | B2051 | | 9.555 | 7.288 | 31.324 | 1.00 21.56 | С |
| ATOM | 1298 | | | B2051 | | 10.708 | 7.230 | 32.106 | 1.00 22.47 | С |
| ATOM | 1299 | CZ | | B2051 | | 10.832 | 6.243 | 33.072 | 1.00 24.14 | С |
| ATOM | 1300 | OH | | B2051 | | 11.973 | 6.182 | 33.843 | 1.00 26.11 | 0 |
| ATOM | 1301 | C | | B2051 | | 7.749 | 4.123 | 29.645 | 1.00 22.35 | С |
| ATOM | 1301 | 0 | | B2051 | | 8.834 | 3.603 | 29.397 | 1.00 21.78 | 0 |
| ATOM | 1302 | N | | B2052 | | 6.735 | 3.470 | 30.200 | 1.00 21.05 | N |
| ATOM | 1303 | CA | | B2052 | | 6.820 | 2.069 | 30.581 | 1.00 20.91 | С |
| ATOM | 1304 | CB | | B2052 | | 5.486 | 1.626 | 31.193 | 1.00 19.71 | С |
| ATOM | 1306 | CG | | B2052 | | 5.321 | 0.141 | 31.535 | 1.00 20.97 | С |
| ATOM | 1300 | | | B2052 | | 6.463 | -0.293 | 32.453 | 1.00 20.68 | С |
| MOTA | 1307 | | | B2052 | • | 3.953 | -0.092 | 32.206 | 1.00 18.56 | С |
| ATOM | 1309 | C | | B2052 | | 7.176 | 1.164 | 29.394 | 1.00 19.19 | С |
| ATOM | 1310 | Ö | | B2052 | | 8.055 | 0.305 | 29.502 | 1.00 18.65 | 0 |
| ATOM | 1311 | N | | B2052 | | 6.501 | 1.365 | 28.264 | 1.00 18.96 | N |
| ATOM | 1312 | CA | | B2053 | | 6.748 | 0.553 | 27.075 | 1.00 18.97 | С |
| ATOM | 1313 | CB | | B2053 | | 5.712 | 0.867 | 26.003 | 1.00 19.24 | С |
| ATOM | 1314 | C | | B2053 | | 8.153 | 0.777 | 26.526 | 1.00 19.65 | С |
| ATOM | 1315 | Ö | | B2053 | | 8.811 | -0.167 | 26.067 | 1.00 19.77 | 0 |
| MOTA | 1316 | N | | B2054 | | 8.604 | 2.028 | 26.569 | 1.00 18.25 | N |
| ATOM | 1317 | CA | | B2054 | | 9.930 | 2.355 | 26.084 | 1.00 16.89 | С |
| ATOM | 1318 | C | | B2054 | | 11.004 | 1.748 | 26.970 | 1.00 18.42 | С |
| ATOM | 1319 | Ō | | B2054 | | 12.072 | 1.344 | 26.488 | 1.00 17.94 | 0 |
| ATOM | 1320 | N | | B2055 | | 10.731 | 1.692 | 28.270 | 1.00 16.40 | N |
| ATOM | 1321 | CA | | B2055 | | 11.684 | 1.112 | 29.202 | 1.00 19.09 | С |
| ATOM | 1322 | CB | | B2055 | | 11.253 | -1.377 | 30.647 | 1.00 20.94 | С |
| ATOM | 1323 | CG | | B2055 | | 12.060 | 2:478 | 31.329 | 1.00 20.89 | С |
| ATOM | 1324 | CD | | B2055 | | 11.968 | 3.790 | 30.570 | 1.00 24.51 | C |
| ATOM | 1325 | NE | | B2055 | | 12.987 | 4.745 | 31.003 | 1.00 25.33 | N |
| ATOM | 1326 | CZ | | B2055 | | 13.239 | 5.897 | 30.388 | 1.00 25.95 | С |
| ATOM | 1327 | | | B2055 | | 12.544 | 6.243 | 29.313 | 1.00 23.97 | N |
| MOTA | 1328 | | | B2055 | | 14.194 | 6.700 | 30.843 | 1.00 25.82 | N |
| MOTA | 1329 | C | | B2055 | | 11.774 | -0.386 | 28.932 | 1.00 18.98 | C |
| ATOM | 1330 | Ö | | B2055 | | 12.855 | -0.971 | 28.985 | 1.00 18.90 | 0 |
| ATOM | 1331 | N | | P.B2056 | | 10.632 | -1.003 | 28.631 | 1.00 20.10 | N |
| ATOM | 1332 | CA | | B2056 | | 10.613 | -2.426 | 28.322 | 1.00 20.52 | С |
| | -002 | | | | | | | | | |

| ATOM | 1333 | CB | TRP | B2056 | | 9.178 | -2.930 | 28.107 | 1.00 22.74 | С |
|--------|------|-----|-----|---------|---|--------|------------------|------------------|------------|---|
| ATOM | 1334 | CG | TRP | B2056 | | 9.118 | -4.394 | 27.738 | 1.00 26.17 | С |
| ATOM | 1335 | CD2 | TRP | B2056 | | 8.573 | -5.459 | 28.52 7 | 1.00 27.99 | С |
| ATOM | 1336 | CE2 | TRP | B2056 | | 8.791 | -6.661 | 27.815 | 1.00 28.39 | С |
| ATOM | 1337 | CE3 | TRP | B2056 | | 7.924 | ~5.516 | 29.767 | 1.00 27.60 | С |
| ATOM | 1338 | CD1 | TRP | B2056 | | 9.623 | -4.978 | 26.607 | 1.00 26.87 | С |
| ATOM | 1339 | NE1 | TRP | B2056 | | 9.432 | -6.337 | 26.648 | 1.00 29.27 | N |
| MOTA | 1340 | CZ2 | TRP | B2056 | | 8.384 | -7.906 | 28.301 | 1.00 29.62 | С |
| ATOM | 1341 | | | B2056 | | 7.516 | -6.760 | 30.253 | 1.00 30.44 | С |
| ATOM | 1342 | | | B2056 | | 7.750 | -7.937 | 29.519 | 1.00 30.93 | С |
| ATOM | 1343 | С | | B2056 | | 11.430 | -2.659 | 27.056 | 1.00 18.69 | С |
| ATOM | 1344 | o | | B2056 | • | 12.265 | -3.562 | 27.007 | 1.00 15.35 | 0 |
| ATOM | 1345 | N | | B2057 | | 11.190 | -1.843 | 26.032 | 1.00 18.10 | N |
| ATOM | 1346 | CA | | B2057 | | 11.925 | -1.993 | 24.778 | 1.00 19.73 | С |
| ATOM · | 1347 | СВ | | B2057 | | 11.475 | -0.948 | 23.756 | 1.00 21.79 | С |
| ATOM | 1348 | OG | | B2057 | | 10.174 | -1.245 | 23.273 | 1.00 30.44 | 0 |
| ATOM | 1349 | C | | B2057 | | 13.427 | -1.857 | 25.009 | 1.00 17.21 | С |
| ATOM | 1350 | 0 | | B2057 | | 14.207 | -2.679 | 24.539 | 1.00 17.96 | 0 |
| ATOM | 1351 | N | | B2058 | | 13.821 | -0.814 | 25.728 | 1.00 15.24 | N |
| ATOM | 1352 | CA | | B2058 | | 15.233 | -0:568 | 26.016 | 1.00 15.12 | C |
| | 1353 | CB | | B2058 | | 15.387 | 0.718 | 26.819 | 1.00 14.34 | C |
| ATOM | 1354 | С | | B2058 | | 15.879 | -1.724 | 26.768 | 1.00 15.45 | Ċ |
| ATOM | | | | B2058 | | 16.981 | -2.158 | 26.421 | 1.00 14.80 | ō |
| ATOM | 1355 | 0 | | | | 15.203 | -2.216 | 27.804 | 1.00 15.14 | N |
| ATOM | 1356 | N | | B2059 | | 15.748 | -3.315 | 28.593 | 1.00 16.97 | C |
| ATOM | 1357 | CA | | B2059 | | 14.909 | -3.523 | 29.860 | 1.00 18.38 | č |
| ATOM | 1358 | CB | | B2059 | | 14.958 | -2.303 | 30.796 | 1.00 17.80 | Ċ |
| ATOM | 1359 | CG | | B2059 | | | -2.546 | 32.097 | 1.00 17.00 | Ċ |
| ATOM | 1360 | CD | | B2059 | | 14.216 | | 33.021 | 1.00 19.57 | Ċ |
| ATOM | 1361 | CE | | B2059 | | 14.345 | -1.327 -1.624 | 34.417 | 1.00 19.37 | N |
| ATOM | 1362 | NZ | | B2059 | | 13.932 | | 27.792 | 1.00 20.44 | C |
| ATOM | 1363 | C | | B2059 | | 15.857 | -4.608 | 27.752 | 1.00 17.35 | Ö |
| ATOM | 1364 | 0 | | B2059 | | 16.805 | -5.375 | 26.904 | 1.00 17.88 | N |
| MOTA | 1365 | N | | B2060 | | 14.897 | -4.844 | | 1.00 17.83 | C |
| MOTA | 1366 | CA | | B2060 | | 14.923 | -6.041 | 26.070 25.420 | 1.00 17.87 | C |
| ATOM | 1367 | CB | | B2060 | | 13.551 | -6.261 | 24.361 | 1.00 13.30 | Č |
| ATOM | 1368 | CG | | B2060 | | 13.519 | -7.359 | | 1.00 23.02 | Ċ |
| ATOM | 1369 | CD | | B2060 | | 13.834 | -8.753 | 24.897 26.099 | 1.00 24.90 | 0 |
| ATOM | 1370 | | | B2060 | | 14.150 | -8.906 | | 1.00 27.02 | 0 |
| MOTA | 1371 | | | B2060 | | 13.764 | -9.707 | 24.096 | 1.00 27.02 | C |
| ATOM | 1372 | C | | B2060 | | 16.013 | -5.885 | 24.999 | 1.00 17.82 | Ö |
| ATOM | 1373 | 0 | | B2060 | | 16.769 | -6.816 | 24.741 | 1.00 15.73 | N |
| ATOM | 1374 | N | | B2061 | | 16.106 | -4.700 | 24.396 | 1.00 15.33 | C |
| ATOM | 1375 | CA | | B2061 | | 17.126 | -4.443 | 23.379 22.868 | 1.00 13.22 | Č |
| ATOM | 1376 | CB | | B2061 | | 17.017 | -3.010 | | 1.00 12.03 | C |
| MOTA | 1377 | | | B2061 | | | | 23.337 | 1.00 15.43 | 0 |
| ATOM | 1378 | 0 | | B2061 | | 19.396 | -5.252 | 25.227 | | N |
| ATOM | 1379 | N | | E B2062 | | 18.699 | | | 1.00 15.78 | c |
| ATOM | 1380 | CA | | E B2062 | | 19.965 | -4:441 | 25.923 | 1.00 18.34 | c |
| MOTA | 1381 | CB | | E B2062 | | 19.972 | -3.664 | 27.244 | 1.00 20.05 | c |
| MOTA | 1382 | CG | | E B2062 | | 21.173 | -3.954 | 28.110 | 1.00 20.65 | c |
| ATOM | 1383 | | | E B2062 | | 21.180 | -5.055 | 28.972 | | C |
| MOTA | 1384 | | | E B2062 | | 22.311 | -3.158 | 28.030 | | C |
| MOTA | 1385 | | | E B2062 | | 22.304 | -5.358 | 29.737 | | c |
| MOTA | 1386 | | | E B2062 | | 23.450 | | | | C |
| ATOM | 1387 | | | E B2062 | | 23.443 | | | | C |
| ATOM | 1388 | C | | E B2062 | | 20.210 | | | - | 0 |
| ATOM | 1389 | 0 | PHI | E B2062 | | 21.297 | -6.455 | 25.933 | 1.00 17.00 | 9 |

| ATOM | 1390 | N | SER | B2063 | 19.203 | -6.608 | 26.730 | 1.00 18. | 58 | | N |
|------|------|-----|-----|-------|--------|---------|--------|----------|-----|---|------|
| ATOM | 1391 | CA | SER | B2063 | 19.336 | -8.033 | 27.016 | 1.00 19. | 54 | | С |
| MOTA | 1392 | CB | SER | B2063 | 18.025 | -8.584 | 27.565 | 1.00 19. | 74 | | С |
| ATOM | 1393 | OG | SER | B2063 | 17.710 | -7.950 | 28.793 | 1.00 22. | 28 | | 0 |
| ATOM | 1394 | С | SER | B2063 | 19.733 | -8.789 | 25.753 | 1.00 20. | 63 | | С |
| ATOM | 1395 | 0 | | B2063 | 20.574 | -9.682 | 25.803 | 1.00 18. | 71 | | 0 |
| ATOM | 1396 | N | | B2064 | 19.128 | -8.430 | 24.620 | 1.00 19. | 41 | | N |
| ATOM | 1397 | CA | | B2064 | 19.457 | -9.088 | 23.362 | 1.00 20. | | | С |
| ATOM | 1398 | | | B2064 | 18.447 | -8.705 | 22.276 | 1.00 21. | | | C |
| ATOM | 1399 | CG | | B2064 | 17.036 | -9.246 | 22.553 | 1.00 21. | | | C |
| ATOM | 1400 | CD | | B2064 | 16.007 | -8.785 | 21.525 | 1.00 21. | | | Ċ |
| ATOM | 1401 | CE | | B2064 | 16.378 | -9.233 | 20.116 | 1.00 19. | | | C |
| ATOM | 1402 | NZ | | B2064 | 15.400 | -8.764 | 19.091 | 1.00 19. | | | N |
| ATOM | 1403 | C | | B2064 | 20.875 | -8.709 | 22.946 | 1.00 20. | | | C |
| ATOM | 1404 | ō | | B2064 | 21.573 | -9.498 | 22.310 | 1.00 21. | | | 0 |
| ATOM | 1405 | N | | B2065 | 21.303 | -7.502 | 23.308 | 1.00 17. | | | Ň |
| ATOM | 1405 | CA | | B2065 | 22.660 | -7.059 | 22.995 | 1.00 19. | | | C |
| ATOM | 1407 | CB | | B2065 | 22.826 | -5.576 | 23.323 | 1.00 15. | | | C |
| ATOM | 1407 | C | | B2065 | 23.647 | -7.892 | 23.820 | 1.00 20 | | | Č |
| | | 0 | | B2065 | 24.793 | -8.096 | 23.414 | 1.00 18 | | | Õ |
| MOTA | 1409 | | | | | -8.359 | 24.985 | 1.00 22 | | | N |
| ATOM | 1410 | N | | B2066 | 23.199 | | | 1.00 27 | | | C |
| ATOM | 1411 | CA | | B2066 | 24.039 | -9.187 | 25.849 | 1.00 27 | | | C |
| ATOM | 1412 | CB | | B2066 | 23.608 | -9.069 | 27.310 | 1.00 27 | | | |
| ATOM | 1413 | CG | | B2066 | 23.933 | -7.749 | 27.971 | | | | C |
| ATOM | 1414 | SD | | B2066 | 25.678 | -7.548 | 28.342 | 1.00 35 | | | s ·· |
| ATOM | 1415 | CE | | B2066 | 25.840 | -8.691 | 29.727 | 1.00 35 | | | С |
| ATOM | 1416 | C | | B2066 | | -10.646 | 25.416 | 1.00 28 | | | C |
| ATOM | 1417 | 0 | | B2066 | | -11.517 | 25.990 | 1.00 29 | | | 0 |
| ATOM | 1418 | N | | B2067 | | -10.906 | 24.411 | 1.00 30 | | | N |
| ATOM | 1419 | CA | | B2067 | | -12.266 | 23.924 | 1.00 32 | | | С |
| ATOM | 1420 | С | | B2067 | | -13.073 | 24.577 | 1.00 33 | | | С |
| MOTA | 1421 | 0 | | B2067 | | -14.282 | 24.353 | 1.00 35 | | | 0 |
| MOTA | 1422 | N | | B2068 | | -12.425 | 25.369 | 1.00 33 | | | N |
| ATOM | 1423 | CA | | B2068 | | -13.124 | 26.048 | 1.00 35 | | | C |
| ATOM | 1424 | CB | | B2068 | | -13.393 | 27528 | 1.00 37 | | | C |
| ATOM | 1425 | OG1 | | B2068 | | -12.149 | 28.194 | 1.00 37 | | | 0 |
| ATOM | 1426 | CG2 | | B2068 | | -14.274 | 27.622 | 1.00 40 | | | С |
| MOTA | 1427 | C | | B2068 | | -12.396 | 26.008 | 1.00 34 | | | C |
| MOTA | 1428 | 0 | | B2068 | | -11.679 | 25.054 | 1.00 34 | | | 0 |
| ATOM | 1429 | N | | B2069 | | -12.598 | 27.051 | 1.00 34 | | | N |
| ATOM | 1430 | CA | | B2069 | | -11.970 | 27.132 | 1.00 33 | | | C |
| MOTA | 1431 | C | | B2069 | | -11.248 | 28.452 | 1.00 33 | | | C |
| ATOM | 1432 | 0 | | B2069 | | -11.590 | 29.455 | 1.00 32 | | | 0 |
| ATOM | 1433 | N | | B2070 | | -10.263 | 28.467 | 1.00 33 | | | N |
| ATOM | 1434 | CA | | B2070 | 15.059 | | 29.680 | 1.00 34 | | | C |
| ATOM | 1435 | CB | | B2070 | 14.122 | | 29.401 | 1.00 33 | | | C |
| ATOM | 1436 | | | B2070 | 12.761 | | 28.904 | 1.00 35 | | | С |
| ATOM | 1437 | | | B2070 | 13.966 | | 30.672 | 1.00 32 | | | С |
| ATOM | 1438 | | | B2070 | 15.277 | | 31.269 | 1.00 28 | | | C |
| MOTA | 1439 | C | | B2070 | | -10.295 | 30.856 | 1.00 35 | | • | С |
| ATOM | 1440 | 0 | | B2070 | | -10.039 | 32.008 | 1.00 35 | | | 0 |
| ATOM | 1441 | N | | B2071 | | -11.276 | 30.572 | 1.00 37 | | | N |
| ATOM | 1442 | CA | | B2071 | | -12.104 | 31.630 | 1.00 39 | | | C |
| ATOM | 1443 | CB | | B2071 | | -13.025 | 31.066 | 1.00 42 | | | C |
| ATOM | 1444 | OG | | B2071 | | -13.795 | 32.102 | 1.00 46 | | | 0 |
| ATOM | 1445 | C | | B2071 | | -12.947 | 32.299 | 1.00 40 | | | C |
| ATOM | 1446 | 0 | SER | B2071 | 14.024 | -13.402 | 33.428 | 1.00 39 | .81 | | 0 |
| | | | | | | | | | | | |

| ATOM | 1447 | N | LYS | B2072 | 15.299 | -13.154 | 31.596 | 1.00 39.77 | N |
|------|------|-----|-----|----------------|--------|---------|--------|--------------------------|--------|
| ATOM | 1448 | CA | LYS | B2072 | 16.403 | -13.940 | 32.132 | 1.00 39.15 | С |
| ATOM | 1449 | CB | LYS | B2072 | 17.115 | -14.689 | 31.007 | 1.00 40.68 | С |
| ATOM | 1450 | | LYS | B2072 | 16.225 | -15.656 | 30.252 | 1.00 43.38 | С |
| ATOM | 1451 | | LYS | B2072 | 16.996 | -16.371 | 29.151 | 1.00 44.69 | С |
| ATOM | 1452 | CE | | B2072 | 16.070 | | 28.342 | 1.00 46.81 | С |
| ATOM | 1453 | NZ | | B2072 | 15.337 | | 29.214 | 1.00 47.85 | N |
| ATOM | 1454 | | | B2072 | 17.396 | | 32.842 | 1.00 38.30 | C |
| ATOM | 1455 | 0 | | B2072 | 17.952 | | 33.879 | 1.00 38.50 | 0 |
| ATOM | 1456 | N | | B2073 | 17.613 | | 32.269 | 1.00 36.74 | N |
| ATOM | 1457 | CA | | B2073 | | -10.883 | 32.821 | 1.00 34.89 | C |
| ATOM | 1458 | CB | | B2073 | 18.817 | -9.803 | 31.766 | 1.00 35.18 | Ċ |
| ATOM | 1459 | CG | | B2073 | 20.010 | -8.856 | 31.910 | 1.00 35.71 | Ċ |
| MOTA | 1460 | | | B2073 | 19.804 | -7.943 | 33.107 | 1.00 37.71 | c |
| | | | | B2073 | 21.296 | -9.661 | 32.050 | 1.00 36.74 | č |
| MOTA | 1461 | | | B2073 | | -10.259 | 34.098 | 1.00 34.21 | c |
| MOTA | 1462 | C | | | | -10.233 | 35.071 | 1.00 34.21 | o |
| ATOM | 1463 | 0 | | B2073 B2074 | 16.658 | -9.982 | 34.090 | 1.00 33.08 | N |
| ATOM | 1464 | N | | | | -9.383 | 35.247 | 1.00 33.00 | C |
| ATOM | 1465 | CA | | B2074 | 16.014 | | | 1.00 30.96 | č |
| MOTA | 1466 | С | | B2074 | 15.762 | -7.897 | 35.053 | 1.00 30.30 | 0 |
| MOTA | 1467 | 0 | | B2074 | 16.702 | -7.127 | 34.871 | | |
| MOTA | 1468 | N | | B2075 | 14.497 | -7.489 | 35.095 | 1.00 29.97 1.00 30.52 | N C |
| MOTA | 1469 | CA | | B2075 | 14.139 | -6.083 | 34.913 | | c |
| MOTA | 1470 | CB | | B2075 | 12.620 | -5.896 | 34.973 | 1.00 32.55 | c |
| MOTA | 1471 | CG | | B2075 | 11.880 | -6.511 | 33.822 | 1.00 33.89 | c |
| MOTA | 1472 | | | B2075 | 11.474 | -7.843 | 33.868 | 1.00 35.06 | |
| ATOM | 1473 | | | B2075 | 11.578 | -5.755 | 32.693 | 1.00 34.72 | С |
| MOTA | 1474 | | | B2075 | 10.774 | -8.412 | 32.806 | 1.00 35.34 | C |
| MOTA | 1475 | | | B2075 | 10.879 | -6.316 | 31.623 | 1.00 34.77 | C |
| MOTA | 1476 | CZ | | B2075 | 10.477 | -7.646 | 31.681 | 1.00 34.64 | C |
| MOTA | 1477 | С | | B2075 | 14.769 | -5.146 | 35.934 | 1.00 29.45 | С |
| MOTA | 1478 | 0 | | B2075 | 15.159 | -4.025 | 35.599 | 1.00 30.37 | 0 |
| MOTA | 1479 | N | | B2076 | 14.867 | -5.607 | 37.177 | 1.00 28.05 | N |
| MOTA | 1480 | CA | | B2076 | 15.417 | -4.796 | 38.259 | 1.00 27.24 | С |
| ATOM | 1481 | CB | GLN | B2076 | 15.043 | -5.420 | 39.607 | 1.00 27.56 | C |
| ATOM | 1482 | CG | | B2076 | 13.539 | -5.436 | 39.859 | 1.00 27.74 | C |
| MOTA | 1483 | CD | | B2076 | 12.929 | -4.041 | 39.834 | 1.00 30.00 | C |
| MOTA | 1484 | OE1 | GLN | B2076 | 11.896 | -3.807 | 39.193 | 1.00 31.13 | 0 |
| MOTA | 1485 | NE2 | GLN | B2076 | 13.563 | -3.107 | 40.536 | 1.00 28.51 | N |
| MOTA | 1486 | С | | B2076 | 16.920 | -4.538 | 38.198 | 1.00 26.61 | C |
| MOTA | 1487 | 0 | | B2076 | 17.430 | -3.698 | 38.935 | 1.00 25.98 | 0 |
| MOTA | 1488 | N | | B2077 | 17.621 | -5.251 | 37.320 | 1.00 26.64 | И |
| MOTA | 1489 | CA | | B2077 | | -5.084 | 37.160 | 1.00 27.59 | C |
| MOTA | 1490 | CB | | B2077 | 19.723 | -6.426 | 36.847 | 1.00 32.09 | C |
| MOTA | 1491 | CG | | B2077 | 19.749 | -7.352 | 38.041 | 1.00 35.66 | C |
| ATOM | 1492 | OD1 | ASP | B2077 | 18.670 | -7.841 | 38.440 | 1.00 39.93 | 0 |
| ATOM | 1493 | OD2 | | B2077 | 20.850 | -7.584 | 38.586 | 1.00 40.87 | 0 |
| MOTA | 1494 | С | ASP | B2077 | 19.403 | -4.087 | 36.054 | 1.00 26.77 | C |
| MOTA | 1495 | 0 | | B2077 | 20.571 | -3.825 | 35.779 | 1.00 25.66 | 0 |
| ATOM | 1496 | N | | B2078 | 18.375 | -3.539 | 35.420 | 1.00 24.12 | N |
| MOTA | 1497 | CA | LEU | B2078 | 18.570 | -2.571 | 34.356 | 1.00 23.25 | C |
| MOTA | 1498 | CB | LEU | B2078 | 18.058 | -3.118 | 33.018 | 1.00 23.97 | С |
| ATOM | 1499 | CG | LEU | B2078 | 18.750 | -4.370 | 32.475 | 1.00 24.92 | C |
| ATOM | 1500 | CD1 | LEU | B2078 | 17.987 | -4.914 | 31.276 | 1.00 23.04 | C |
| MOTA | 1501 | CD2 | | B2078 | 20.180 | -4.021 | 32.089 | 1.00 26.74 | С |
| ATOM | 1502 | С | LEU | B2078 | 17.795 | -1.321 | 34.702 | 1.00 23.29 | C |
| ATOM | 1503 | 0 | LEU | B2078 | 16.669 | -1.390 | 35.196 | 1.00 23.17 | 0 |
| | | | | | | | | | |

| ATOM | 1504 | N | GLU | B2079 | 18.397 | -0.173 | 34.446 | 1.00 21.42 | N |
|--------------|--------------|----------|-----|---|--------|--------|--------|------------|---|
| MOTA | 1505 | CA | GLU | B2079 | 17.724 | 1.075 | 34.716 | 1.00 21.45 | C |
| MOTA | 1506 | CB | GLU | B2079 | 18.192 | 1.666 | 36.036 | 1.00 22.77 | С |
| ATOM | 1507 | CG | GLU | B2079 | 17.346 | 2.835 | 36.477 | 1.00 24.03 | С |
| ATOM | 1508 | CD | GLU | B2079 | 17.726 | 3.340 | 37.848 | 1.00 25.73 | С |
| MOTA | 1509 | OE1 | GLU | B2079 | 18.797 | 3.972 | 37.976 | 1.00 26.42 | 0 |
| MOTA | 1510 | | | B2079 | 16.950 | 3.099 | 38.798 | 1.00 27.63 | 0 |
| ATOM | 1511 | C | | B2079 | 18.014 | 2.055 | 33.600 | 1.00 20.55 | С |
| ATOM | 1512 | 0 | | B2079 | 19.167 | 2.241 | 33.203 | 1.00 20.96 | 0 |
| ATOM | 1513 | N | | B2080 | 16.954 | 2.666 | 33.095 | 1.00 18.00 | N |
| ATOM | 1514 | CA | | B2080 | 17.055 | 3.648 | 32.033 | 1.00 18.55 | С |
| ATOM | 1515 | СВ | | B2080 | 16.268 | 3.211 | 30.769 | 1.00 16.14 | С |
| ATOM | 1516 | | | B2080 | 16.429 | 4.262 | 29.686 | 1.00 16.12 | С |
| ATOM | 1517 | | | B2080 | 16.755 | 1.849 | 30.276 | 1.00 14.67 | С |
| ATOM | 1518 | C | | B2080 | 16.442 | 4.948 | 32.549 | 1.00 19.85 | С |
| ATOM | 1519 | ŏ | | B2080 | 15.234 | 5.019 | 32.805 | 1.00 19.59 | 0 |
| ATOM | 1520 | N | | B2081 | 17.279 | 5.966 | 32.708 | 1.00 20.39 | N |
| ATOM | 1521 | CA | | B2081 | 16.825 | 7.271 | 33.176 | 1.00 21.24 | С |
| ATOM | 1522 | CB | | B2081 | 17.644 | 7.716 | 34.394 | 1.00 21.31 | С |
| ATOM | 1523 | CG | | B2081 | 17.683 | 6.758 | 35.593 | 1.00 22.71 | C |
| ATOM | 1524 | | | B2081 | 18.641 | 7.299 | 36.661 | 1.00 23.10 | C |
| ATOM | 1525 | | | B2081 | 16.280 | 6.594 | 36.165 | 1.00 22.25 | Č |
| ATOM | 1526 | C | | B2081 | 17.027 | 8.259 | 32.040 | 1.00 22.16 | c |
| ATOM | 1527 | o | | B2081 | 17.421 | 7.882 | 30.934 | 1.00 22.05 | Ō |
| ATOM | 1528 | Ŋ | | B2081 | 16.755 | 9.526 | 32.309 | 1.00 22.54 | N |
| ATOM | 1529 | CA | | B2082 | 16.933 | 10.561 | 31.303 | 1.00 24.30 | C |
| | | CB | | B2082 | 15.598 | 11.247 | 31.022 | 1.00 25.64 | C |
| ATOM | 1530 1531 | CG | | B2082 | 14.657 | 10.371 | 30.207 | 1.00 27.22 | c |
| MOTA | | | | B2082 | 14.779 | 10.371 | 28.982 | 1.00 28.88 | Ö |
| ATOM | 1532 1533 | | | B2082 | 13.729 | 9.710 | 30.883 | 1.00 24.27 | N |
| MOTA MOTA | 1534 | C | | B2082 | 17.945 | 11.555 | 31.840 | 1.00 25.00 | c C |
| | | | | B2082 | 17.860 | 11.958 | 33.001 | 1.00 23.46 | Ö |
| ATOM ATOM | 1535 1536 | O N | | B2083 | 18.913 | 11.939 | 31.010 | 1.00 25.22 | N |
| | 1537 | | | B2083 | 19.920 | 12.890 | 31.454 | 1.00 25.69 | C |
| ATOM | | CA | | B2083 | 21.215 | 12.744 | 30.641 | 1.00 25.99 | Ċ |
| ATOM ATOM | 1538 1539 | CB CG | | B2083 | 21.013 | 12.744 | 29.153 | 1.00 27.46 | Č |
| ATOM | 1540 | | | B2083 | 20.173 | 13.758 | 28.729 | 1.00 25.62 | Ö |
| ATOM | 1541 | | | B2083 | 21.811 | 12.265 | 28.348 | 1.00 27.23 | . N |
| ATOM | 1542 | C | | B2083 | 19.410 | 14.330 | 31.397 | 1.00 26.79 | C |
| ATOM | 1543 | 0 | | B2083 | 18.216 | 14.571 | 31.215 | 1.00 25.77 | ō |
| ATOM | 1544 | N | | B2084 | 20.322 | 15.281 | 31.559 | 1.00 29.60 | N |
| ATOM | 1545 | CA | | B2084 | 19.982 | 16.701 | 31.563 | 1.00 31.78 | C |
| ATOM | 1546 | CB | | B2084 | 21.238 | 17.539 | 31.827 | 1.00 33.94 | С |
| MOTA | 1547 | CG | | B2084 | 22.148 | 16.960 | 32.896 | 1.00 39.23 | Ċ |
| ATOM | 1548 | CD | | B2084 | 22.774 | | 32.470 | | C |
| MOTA | 1549 | | | B2084 | 23.642 | 15.652 | 31.567 | 1.00 42.45 | 0 |
| ATOM | 1550 | | | B2084 | 22.390 | 14.588 | 33.030 | 1.00 42.21 | 0 |
| ATOM | 1551 | C | | B2084 | 19.351 | 17:153 | 30.253 | 1.00 30.81 | С |
| MOTA | 1552 | 0 | | B2084 | 18.472 | 18.013 | 30.242 | 1.00 29.26 | 0 |
| ATOM | 1553 | N | | B2085 | 19.808 | 16.573 | 29.148 | 1.00 30.86 | N |
| ATOM | 1554 | CA | | B2005 | 19.291 | 16.940 | 27.838 | 1.00 31.05 | c |
| ATOM | 1555 | CB | | B2085 | 20.364 | 16.716 | 26.775 | 1.00 33.27 | C |
| ATOM | 1556 | CG | | B2085 | 21.598 | 17.554 | 27.005 | 1.00 35.81 | c |
| ATOM | 1557 | CD | | B2085 | 22.636 | 17.335 | 25.928 | 1.00 38.24 | C |
| ATOM | 1558 | NE | | B2085 | 23.735 | 18.286 | 26.060 | 1.00 41.03 | N |
| ATOM | 1559 | | | B2085 | 24.544 | 18.349 | 27.110 | 1.00 42.41 | С |
| ATOM | 1560 | | | B2085 | 24.381 | 17.515 | 28.128 | 1.00 43.26 | N |
| WI OLI | 1000 | .411.4 | | , ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | 24.501 | 1 | | 2.25 .0.20 | • |

| | | | | | | | | | NT |
|--------|------|-----|-----|----------|--------|---------|--------|------------|----|
| MOTA | 1561 | NH2 | ARG | B2085 | 25.523 | 19.239 | 27.138 | 1.00 44.30 | N |
| MOTA | 1562 | С | ARG | B2085 | 18.024 | 16.190 | 27.465 | 1.00 30.14 | C |
| ATOM | 1563 | 0 | ARG | B2085 | 17.450 | 16.432 | 26.408 | 1.00 31.11 | 0 |
| ATOM | 1564 | N | | B2086 | 17.593 | 15.273 | 28.326 | 1.00 29.20 | N |
| ATOM | 1565 | CA | | B2086 | 16.371 | 14.530 | 28.057 | 1.00 27.93 | С |
| | 1566 | C | | B2086 | 16.531 | 13.222 | 27.304 | 1.00 26.69 | С |
| MOTA | | | | | 15.541 | 12.581 | 26.952 | 1.00 27.22 | 0 |
| ATOM | 1567 | 0 | | B2086 | | 12.818 | 27.056 | 1.00 24.98 | N |
| MOTA | 1568 | N | | B2087 | 17.770 | | 26.340 | 1.00 23.11 | C |
| ATOM | 1569 | CA | | B2087 | 18.033 | 11.582 | | 1.00 23.11 | c |
| ATOM | 1570 | CB | | B2087 | 19.358 | 11.692 | 25.589 | | Ċ |
| ATOM | 1571 | С | ALA | B2087 | 18.065 | 10.369 | 27.269 | 1.00 22.69 | |
| MOTA | 1572 | 0 | ALA | B2087 | 18.611 | 10.431 | 28.370 | 1.00 22.81 | 0 |
| ATOM | 1573 | N | PRO | B2088 | 17.481 | 9.242 | 26.833 | 1.00 22.85 | N |
| MOTA | 1574 | CD | PRO | B2088 | 16.722 | 9.014 | 25.588 | 1.00 23.63 | C |
| ATOM | 1575 | CA | PRO | B2088 | 17.485 | 8.039 | 27.674 | 1.00 21.17 | С |
| ATOM | 1576 | CB | PRO | B2088 | 16.471 | 7.134 | 26.982 | 1.00 22.95 | С |
| ATOM | 1577 | CG | | B2088 | 16.650 | 7.489 | 25.528 | 1.00 24.16 | С |
| ATOM | 1578 | C | | B2088 | 18.879 | 7.416 | 27.716 | 1.00 20.46 | С |
| | 1579 | 0 | | B2088 | 19.584 | 7.407 | 26.712 | 1.00 18.12 | 0 |
| ATOM | | | | B2089 | 19.280 | 6.906 | 28.878 | 1.00 19.76 | N |
| ATOM | 1580 | N | | | 20.593 | 6.275 | 29.019 | 1.00 19.97 | С |
| MOTA | 1581 | CA | | B2089 | 21.660 | | 29.324 | 1.00 20.30 | С |
| MOTA | 1582 | CB | | B2089 | | | 30.743 | 1.00 21.25 | Č |
| ATOM | 1583 | CG | | B2089 | 21.605 | 7.850 | | 1.00 21.25 | č |
| MOTA | 1584 | | | B2089 | 22.471 | 7.347 | 31.719 | | c |
| ATOM | 1585 | | | B2089 | 22.386 | 7.765 | 33.046 | 1.00 22.62 | C |
| ATOM | 1586 | | | B2089 | 20.651 | | 31.128 | 1.00 21.67 | |
| ATOM | 1587 | CE2 | TYR | B2089 | 20.557 | 9.218 | 32.454 | 1.00 23.51 | C |
| ATOM | 1588 | CZ | TYR | B2089 | 21.429 | 8.693 | 33.404 | 1.00 22.23 | C |
| ATOM | 1589 | ОН | TYR | B2089 | 21.327 | 9.078 | 34.715 | 1.00 23.91 | 0 |
| ATOM | 1590 | С | TYR | B2089 | 20.547 | 5.246 | 30.148 | 1.00 18.84 | С |
| ATOM | 1591 | Ō | | B2089 | 19.738 | 5.356 | 31.066 | 1.00 16.92 | 0 |
| ATOM | 1592 | Ň | | B2090 | 21.408 | 4.237 | 30.076 | 1.00 19.96 | N |
| ATOM | 1593 | CA | | B2090 | 21.432 | | 31.116 | 1.00 20.18 | C |
| ATOM | 1594 | CB | | B2090 | 22.015 | | 30.588 | 1.00 18.86 | С |
| | 1595 | CG | | B2090 | 21.031 | | 29.813 | 1.00 17.77 | С |
| ATOM | | | | B2090 | 20.843 | | 28.452 | 1.00 18.34 | C |
| ATOM | 1596 | | | B2090 | 20.276 | | 30.455 | 1.00 17.66 | С |
| ATOM | 1597 | | | | 19.915 | | 27.737 | 1.00 16.58 | С |
| MOTA | 1598 | | | B2090 | 19.344 | | 29.751 | 1.00 16.83 | С |
| ATOM | 1599 | | | B2090 | | | 28.393 | 1.00 18.42 | Ċ |
| MOTA | 1600 | CZ | | B2090 | 19.166 | | 32.307 | 1.00 21.96 | Č |
| MOTA | 1601 | C | | E B2090 | 22.249 | | 32.215 | 1.00 21.17 | Ō |
| ATOM | 1602 | | | E B2090 | 23.464 | | | 1.00 21.79 | N |
| ATOM | 1603 | | | R B2091 | 21.569 | | 33.423 | 1.00 21.79 | Ċ |
| MOTA | 1604 | CA | | R B2091 | 22.233 | | 34.642 | | Č |
| MOTA | 1605 | CB | | R B2091 | 21.269 | | 35.498 | | - |
| MOTA | 1606 | OG | | R B2091 | 20.046 | | 35.689 | 1.00 27.15 | 0 |
| ATOM | 1607 | С | | R B2091 | 22.67 | | 35.406 | _ | C |
| ATOM | 1608 | 0 | SE | R B2091 | 23.572 | | 36.241 | | 0 |
| ATOM | 1609 | N | GL | N B2092 | 22.039 | 9 1.974 | 35.100 | | N |
| ATOM | 1610 | | GL | N B2092 | 22.343 | 3 0.702 | 35.750 | | C |
| ATOM | 1611 | | | N B2092 | 21.32 | | 36.858 | | C |
| ATOM | 1612 | | | N B2092 | 21.73 | 8 0.888 | 38.236 | 1.00 36.96 | С |
| ATOM | 1613 | | | N B2092 | 22.79 | | 38.846 | 1.00 41.69 | С |
| ATOM | 1614 | | | N B2092 | 23.92 | | | 1.00 44.08 | 0 |
| . ATOM | 1615 | | | N B2092 | 22.41 | | | | |
| ATOM | 1616 | | | N B2092 | 22.31 | | | | |
| ATOM | 1617 | | | N B2092 | 21.35 | | | | |
| MION | 1011 | ~ | GI. | ., 5.072 | | | | | |

| ATOM | 1618 | N | ALA | B2093 | 23.378 | -1.243 | 34.750 | 1.00 24.06 | N |
|------|------|-----|-----|-------|--------|--------|---------|--------------------------|---|
| ATOM | 1619 | | | B2093 | 23.451 | -2.379 | 33.845 | 1.00 24.55 | С |
| ATOM | 1620 | | | B2093 | 23.544 | -1.896 | 32.401 | 1.00 23.95 | С |
| ATOM | 1621 | | | B2093 | 24.654 | -3.240 | 34.182 | 1.00 24.42 | С |
| ATOM | 1622 | | | B2093 | 25.669 | -2.737 | 34.662 | 1.00 23.73 | 0 |
| ATOM | 1623 | N | | B2094 | 24.542 | -4.560 | 33.958 | 1.00 24.28 | N |
| ATOM | 1624 | CD | | B2094 | 23.286 | -5.266 | 33.634 | 1.00 24.45 | С |
| ATOM | 1625 | CA | | B2094 | 25.625 | -5.509 | 34.228 | 1.00 24.13 | С |
| | 1626 | CB | | B2094 | 24.882 | -6.827 | 34.404 | 1.00 24.53 | С |
| ATOM | 1627 | CG | | B2094 | 23.752 | -6.693 | 33.412 | 1.00 25.43 | Ċ |
| ATOM | 1628 | C | | B2094 | 26.575 | -5.532 | 33.033 | 1.00 25.18 | Ċ |
| ATOM | 1629 | | | B2094 | 26.687 | -6.538 | 32.330 | 1.00 27.39 | 0 |
| ATOM | | 0 | | B2095 | 27.237 | -4.406 | 32.795 | 1.00 25.59 | N |
| MOTA | 1630 | N | | B2095 | 28.166 | -4.276 | 31.674 | 1.00 26.28 | Ċ |
| ATOM | 1631 | CA | | | 27.394 | -3.937 | 30.392 | 1.00 26.01 | č |
| ATOM | 1632 | CB | | B2095 | 28.264 | -3.808 | 29.176 | 1.00 25.16 | c |
| ATOM | 1633 | CG | | B2095 | 28.289 | -2.622 | 28.448 | 1.00 23.33 | Č |
| ATOM | 1634 | | | B2095 | | | 28.766 | 1.00 24.13 | Č |
| ATOM | 1635 | | | B2095 | 29.070 | -4.864 | 27.333 | 1.00 23.09 | C |
| ATOM | 1636 | | | B2095 | 29.106 | -2.488 | | 1.00 24.48 | Ċ |
| ATOM | 1637 | | | B2095 | 29.890 | -4.739 | 27.652 | 1.00 24.48 | C |
| MOTA | 1638 | CZ | | B2095 | 29.906 | -3.542 | 26.933 | | c |
| ATOM | 1639 | C | | B2095 | 29.157 | -3.168 | 32.000 | 1.00 25.62 1.00 26.70 | 0 |
| ATOM | 1640 | 0 | | B2095 | 28.768 | -2.080 | 32.413 | | N |
| ATOM | 1641 | N | | B2096 | 30.438 | | .31.804 | 1.00 26.81 | C |
| MOTA | 1642 | CA | - | B2096 | 31.472 | -2.466 | 32.122 | 1.00 27.94 | C |
| MOTA | 1643 | CB | | B2096 | 32.750 | -3.203 | 32.531 | 1.00 27.66 | |
| ATOM | 1644 | OG | | B2096 | 33.144 | -4.111 | 31.518 | 1.00 29.62 | 0 |
| ATOM | 1645 | С | | B2096 | 31.787 | -1.469 | 31.007 | 1.00 27.71 | С |
| ATOM | 1646 | 0 | | B2096 | 32.430 | -0.452 | 31.249 | 1.00 27.75 | 0 |
| MOTA | 1647 | N | | B2097 | 31.325 | -1.746 | 29.792 | 1.00 26.55 | N |
| ATOM | 1648 | CA | | B2097 | 31.611 | -0.847 | 28.690 | 1.00 23.99 | C |
| MOTA | 1649 | С | | B2097 | 30.611 | 0.274 | 28.499 | 1.00 23.68 | C |
| MOTA | 1650 | 0 | GLY | B2097 | 29.869 | 0.639 | 29.413 | 1.00 22.73 | 0 |
| ATOM | 1651 | N | | B2098 | 30.606 | 0.838 | 27.299 | 1.00 23.32 | N |
| ATOM | 1652 | CA | | B2098 | 29.682 | 1.912 | 26.975 | 1.00 23.52 | C |
| MOTA | 1653 | CB | LYS | B2098 | 30.323 | 2.896 | 25.995 | 1.00 25.66 | С |
| MOTA | 1654 | CG | LYS | B2098 | 31.546 | 3.599 | 26.562 | 1.00 29.30 | С |
| MOTA | 1655 | CD | LYS | B2098 | 32.162 | 4.532 | 25.545 | 1.00 31.81 | C |
| MOTA | 1656 | CE | | B2098 | 33.364 | 5.247 | 26.128 | 1.00 35.72 | C |
| MOTA | 1657 | ΝŻ | | B2098 | 33.970 | 6.194 | 25.154 | 1.00 38.45 | N |
| ATOM | 1658 | С | LYS | B2098 | 28.438 | 1.302 | 26.356 | 1.00 21.94 | C |
| ATOM | 1659 | 0 | | B2098 | 28.518 | 0.350 | 25.570 | 1.00 20.64 | 0 |
| MOTA | 1660 | N | | B2099 | 27.294 | 1.862 | 26.721 | 1.00 20.44 | N |
| MOTA | 1661 | CA | ILE | B2099 | 26.008 | 1.400 | 26.236 | 1.00 19.38 | C |
| ATOM | 1662 | CB | | B2099 | 25.109 | 1.012 | 27.421 | 1.00 19.92 | C |
| MOTA | 1663 | | | B2099 | 23.804 | 0.423 | 26.919 | 1.00 20.26 | C |
| ATOM | 1664 | CG1 | ILE | B2099 | 25.839 | -0.008 | 28.302 | 1.00 19.45 | C |
| MOTA | 1665 | CD1 | ILE | B2099 | 25.193 | -0.230 | 29.663 | 1.00 21.98 | C |
| ATOM | 1666 | С | ILE | B2099 | 25.352 | | 25.444 | 1.00 19.88 | C |
| ATOM | 1667 | 0 | | B2099 | 24.950 | 3.546 | 26.011 | 1.00 19.12 | 0 |
| MOTA | 1668 | N | TRE | B2100 | 25.267 | 2.352 | 24.129 | 1.00 19.02 | Ŋ |
| ATOM | 1669 | CA | | B2100 | 24.662 | 3.351 | 23.265 | 1.00 17.64 | C |
| MOTA | 1670 | CB | TŘE | B2100 | 25.430 | 3.431 | 21.951 | 1.00 19.81 | C |
| MOTA | 1671 | CG | | B2100 | 26.840 | 3.861 | 22.165 | 1.00 20.97 | C |
| MOTA | 1672 | CD2 | TRE | B2100 | 27.295 | 5.202 | 22.383 | 1.00 21.20 | C |
| ATOM | 1673 | CE2 | TRE | B2100 | 28.680 | 5.137 | 22.640 | 1.00 20.87 | С |
| MOTA | 1674 | CE3 | TRE | B2100 | 26.661 | 6.454 | 22.393 | 1.00 22.40 | С |
| | | | | | | | | | |

| ATOM | 1675 | CD1 | TRP | B2100 | 27.93 | 8 3.059 | 22.289 | 1.00 22 | 2.80 | С |
|--------------|------|-----|------|---------|-------|----------|--------|---------|------------|-----|
| ATOM | 1676 | | | B2100 | 29.05 | | 22.576 | 1.00 23 | 1.53 | N |
| ATOM | 1677 | | | B2100 | 29.44 | | 22.901 | 1.00 2 | 1.01 | С |
| ATOM | 1678 | | | B2100 | 27.42 | | 22.654 | 1.00 1 | | С |
| ATOM | 1679 | | | B2100 | 28.80 | | 22.905 | 1.00 2 | 0.24 | C |
| ATOM | 1680 | C | | B2100 | 23.20 | | 23.023 | 1.00 1 | | С |
| ATOM | 1681 | 0 | | B2100 | 22.88 | | 22.308 | 1.00 1 | | Ō |
| ATOM | 1682 | N | | B2101 | 22.32 | | 23.632 | 1.00 1 | | N |
| | | | | B2101 | 20.89 | | 23.524 | 1.00 1 | | C |
| ATOM | 1683 | CA | | B2101 | 20.29 | | 24.925 | 1.00 1 | | Č |
| ATOM | 1684 | CB | | | | | 25.013 | 1.00 1 | | Č |
| ATOM | 1685 | CG | | B2101 | 18.75 | | 24.455 | 1.00 1 | | č |
| ATOM | 1686 | | | B2101 | 18.19 | | 26.467 | 1.00 1 | | C |
| ATOM | 1687 | | | B2101 | 18.32 | | | 1.00 1 | | č |
| MOTA | 1688 | C | | B2101 | 20.14 | | 22.810 | 1.00 1 | | 0 |
| MOTA | 1689 | 0 | | B2101 | 20.46 | | 22.937 | | | N |
| MOTA | 1690 | N | | B2102 | 19.13 | | 22.047 | 1.00 1 | | |
| MOTA | 1691 | CA | | B2102 | 18.26 | | 21.380 | 1.00 1 | | C |
| MOTA | 1692 | CB | | B2102 | 18.68 | | 19.945 | 1.00 1 | | С |
| MOTA | 1693 | OG | | B2102 | 17.85 | | 19.405 | 1.00 1 | | 0 |
| ATOM | 1694 | С | | B2102 | 16.86 | | 21.393 | 1.00 1 | | C |
| MOTA | 1695 | 0 | | B2102 | 16.70 | | 21.230 | 1.00 1 | | 0 |
| ATOM | 1696 | N | ILE | B2103 | 15.86 | 53 5.414 | 21.613 | 1.00 1 | | N |
| MOTA | 1697 | CA | ILE | B2103 | 14.47 | 78 4.948 | 21.646 | 1.00 1 | | С |
| MOTA | 1698 | CB | ILE | B2103 | 13.89 | 5.031 | 23.070 | 1.00 1 | | С |
| MOTA | 1699 | CG2 | ILE | B2103 | 12.43 | 39 4.560 | 23.063 | 1.00 1 | | С |
| MOTA | 1700 | CG1 | ILE | B2103 | 14.76 | 55 4.215 | 24.036 | 1.00 1 | | С |
| ATOM | 1701 | CD1 | ILE | B2103 | 14.40 | 6 4.396 | 25.497 | 1.00 1 | 7.05 | С |
| ATOM | 1702 | С | ILE | B2103 | 13.64 | 5.852 | 20.749 | 1.00 1 | 7.44 | С |
| MOTA | 1703 | 0 | ILE | B2103 | 13.88 | 36 7.055 | 20.684 | 1.00 1 | 7.70 | 0 |
| ATOM | 1704 | N | | B2104 | 12.67 | 75 5.275 | 20,053 | 1.00 1 | 7.76 | N |
| ATOM | 1705 | CA | | B2104 | 11.80 | 03 6.065 | 19.187 | 1.00 1 | 9.81 | С |
| ATOM | 1706 | СВ | | B2104 | 12.35 | | 17.759 | 1.00 1 | 9.27 | С |
| ATOM | 1707 | OG | | B2104 | 11.5 | | 16.930 | 1.00 2 | 0.56 | 0 |
| ATOM | 1708 | C | | B2104 | 10.42 | | 19.189 | 1.00 2 | 0.64 | С |
| ATOM | 1709 | Ö | | B2104 | 10.29 | | 19.338 | 1.00 2 | | 0 |
| ATOM | 1710 | N | | B2105 | 9.39 | | 19.020 | 1.00 2 | 20.13 | N |
| ATOM | 1711 | CA | | B2105 | 8.0 | | 19.028 | 1.00 2 | 22.93 | С |
| ATOM | 1712 | CB | | B2105 | 7.4 | | 20.432 | 1.00 2 | 23.19 | С |
| ATOM | 1713 | CG | | B2105 | 7.2 | | 20.890 | 1.00 2 | 24.84 | С |
| ATOM | 1714 | | | B2105 | 6.2 | | 20.785 | 1.00 2 | | C |
| ATOM | 1715 | | | B2105 | 8.2 | | 21.490 | 1.00 2 | | N |
| ATOM | 1716 | | | B2105 | 7.8 | | 21.737 | 1.00 2 | 25.54 | С |
| ATOM | 1717 | | | B2105 | 6.6 | | 21.318 | 1.00 2 | | N |
| | 1717 | C | | B2105 | 7.1 | | 18.050 | 1.00 2 | | С |
| ATOM | 1719 | 0 | | B2105 | 7.3 | | 17.554 | 1.00 2 | | 0 |
| ATOM ATOM | 1720 | N | | B2106 | 6.0 | | 17.769 | 1.00 | | N |
| | 1721 | CA | | B2106 | 4.9 | | 16.919 | 1.00 | | С |
| ATOM | | CB | | B2106 | 4.6 | | 15.755 | 1.00 | | C |
| ATOM | 1722 | | | R B2106 | 4.2 | | 16.278 | 1.00 | | O |
| ATOM' | 1723 | | | R B2106 | 5.7 | | | 1.00 | | Ċ |
| ATOM | 1724 | | | | 3.7 | | 17.894 | 1.00 | | C |
| ATOM | 1725 | С | | R B2106 | 3.7 | | | 1.00 | | o |
| MOTA | 1726 | 0 | | R B2106 | | | | 1.00 | | N |
| ATOM | 1727 | N | | B2107 | 2.5 | | | 1.00 | | C |
| ATOM | 1728 | CA | | P B2107 | 1.3 | | | 0.05 | | C |
| MOTA | 1729 | CB | | P B2107 | 0.1 | | | 0.05 | | d |
| MOTA | 1730 | CG | | B2107 | 0.1 | | | 0.05 | | 0 |
| ATOM | 1731 | ODI | LASI | P B2107 | 1.0 | 90 9.023 | 17.157 | 0.05 | Z. / . U.L | · · |

| | • | | | | | | | | |
|------|------|-----|-----|---------|--------|--------|--------|------------|--------|
| ATOM | 1732 | OD2 | ASP | B2107 | -0.874 | 8.930 | 18.125 | 0.05 26.97 | 0 |
| ATOM | 1733 | С | ASP | B2107 | 1.085 | 4.877 | 18.788 | 1.00 27.36 | С |
| ATOM | 1734 | 0 | ASP | B2107 | 0.493 | 4.717 | 19.854 | 1.00 29.78 | 0 |
| ATOM | 1735 | N | GLN | B2108 | 1.482 | 3.858 | 18.032 | 1.00 25.07 | N |
| ATOM | 1736 | CA | GLN | B2108 | 1.207 | 2.483 | 18.433 | 1.00 25.09 | C |
| ATOM | 1737 | CB | GLN | B2108 | 0.523 | 1.736 | 17.293 | 1.00 26.05 | С |
| ATOM | 1738 | CG | GLN | B2108 | -0.728 | 2.395 | 16.780 | 1.00 29.37 | С |
| ATOM | 1739 | CD | | B2108 | -1.145 | 1.827 | 15.445 | 1.00 31.53 | С |
| ATOM | 1740 | | | B2108 | -0.362 | 1.822 | 14.492 | 1.00 31.44 | . 0 |
| ATOM | 1741 | | | B2108 | -2.379 | 1.345 | 15.363 | 1.00 31.86 | N |
| ATOM | 1742 | C | | B2108 | 2.412 | 1.658 | 18.876 | 1.00 24.58 | С |
| ATOM | 1743 | Õ | | B2108 | 2.251 | 0.710 | 19.650 | 1.00 22.64 | 0 |
| ATOM | 1744 | N | | B2109 | 3.606 | 2.000 | 18.386 | 1.00 23.20 | N |
| ATOM | 1745 | CA | | B2109 | 4.800 | 1.229 | 18.725 | 1.00 22.81 | С |
| ATOM | 1746 | CB | | B2109 | 5.309 | 0.456 | 17.501 | 1.00 24.68 | С |
| ATOM | 1747 | CG | | B2109 | 4.236 | -0.250 | 16.721 | 1.00 26.08 | С |
| | 1748 | | | B2109 | 3.701 | 0.329 | 15.576 | 1.00 26.47 | С |
| ATOM | 1749 | | | B2109 | 3.783 | -1.505 | 17.110 | 1.00 27.02 | Ċ |
| ATOM | | | | B2109 | 2.729 | -0.336 | 14.825 | 1.00 28.36 | C |
| ATOM | 1750 | | | B2109 | 2.810 | -2.177 | 16.366 | 1.00 27.54 | Č |
| ATOM | 1751 | | | B2109 | 2.287 | -1.592 | 15.224 | 1.00 28.20 | c |
| ATOM | 1752 | CZ | | | | 2.037 | 19.260 | 1.00 21.56 | Č |
| ATOM | 1753 | С | | B2109 | 5.980 | | 19.027 | 1.00 21.30 | Ö |
| ATOM | 1754 | 0 | | B2109 | 6.096 | 3.233 | | 1.00 22.22 | N |
| ATOM | 1755 | N | | B2110 | 6.872 | 1.358 | 19.969 | 1.00 21.04 | C |
| MOTA | 1756 | CA | | B2110 | 8.073 | 2.005 | 20.485 | | C |
| MOTA | 1757 | CB | | B2110 | 7.982 | 2.279 | 22.006 | 1.00 19.74 | C |
| MOTA | 1758 | | | B2110 | 7.649 | 1.001 | 22.751 | 1.00 21.12 | |
| MOTA | 1759 | | | B2110 | 9.307 | 2.861 | 22.504 | 1.00 21.25 | C C |
| MOTA | 1760 | С | | B2110 | 9.230 | 1.063 | 20.197 | 1.00 20.24 | 0 |
| ATOM | 1761 | 0 | | B2110 | 9.160 | -0.128 | 20.523 | 1.00 21.27 | |
| MOTA | 1762 | N | | B2111 | 10.276 | 1.580 | 19.557 | 1.00 19.29 | N |
| MOTA | 1763 | CA | | B2111 | 11.440 | 0.763 | 19.235 | 1.00 20.44 | C |
| MOTA | 1764 | CB | | B2111 | 11.759 | 0.788 | 17.725 | 1.00 22.75 | C |
| ATOM | 1765 | | | B2111 | 12.116 | 2.120 | 17.337 | 1.00 27.12 | 0 |
| ATOM | 1766 | | | B2111 | 10.550 | 0.353 | 16.911 | 1.00 26.61 | C |
| ATOM | 1767 | С | | B2111 | 12.668 | 1.270 | 19.982 | 1.00 19.21 | C |
| ATOM | 1768 | 0 | | B2111 | 12.780 | 2.455 | 20.278 | 1.00 18.06 | 0 |
| MOTA | 1769 | N | | B2112 | 13.581 | 0.353 | 20.280 | 1.00 18.16 | N |
| MOTA | 1770 | CA | | B2112 | 14.810 | 0.675 | 20.988 | 1.00 17.59 | С |
| MOTA | 1771 | CB | | B2112 | 14.715 | 0.231 | 22.442 | 1.00 14.54 | C |
| ATOM | 1772 | С | | B2112 | 15.951 | -0.052 | 20.292 | 1.00 17.15 | С |
| MOTA | 1773 | 0 | | B2112 | 15.776 | -1.163 | 19.788 | 1.00 15.26 | 0 |
| MOTA | 1774 | N | | R B2113 | 17.111 | 0.588 | 20.258 | 1.00 16.75 | N |
| MOTA | 1775 | CA | | R B2113 | 18.297 | 0.015 | 19.631 | 1.00 17.12 | С |
| ATOM | 1776 | CB | | R B2113 | | 0.705 | | 1.00 17.55 | C |
| ATOM | 1777 | OG | | R B2113 | 19.674 | 0.112 | 17.603 | 1.00 19.24 | 0 |
| MOTA | 1778 | С | | R B2113 | 19.470 | .0.227 | 20.588 | 1.00 16.82 | C |
| ATOM | 1779 | 0 | | R B2113 | 19.677 | 1.327 | 21.092 | 1.00 17.25 | 0 |
| MOTA | 1780 | N | | B2114 | 20.220 | -0.837 | 20.840 | 1.00 16.23 | N |
| MOTA | 1781 | CA | | B2114 | 21.364 | -0.778 | 21.736 | 1.00 15.71 | C |
| MOTA | 1782 | CB | | B2114 | 21.129 | | 23.017 | 1.00 13.94 | C |
| ATOM | 1783 | | | B2114 | 22.451 | -1.731 | 23.784 | 1.00 14.11 | C |
| ATOM | 1784 | CG2 | | B2114 | 20.070 | -0.923 | 23.877 | 1.00 10.51 | C |
| MOTA | 1785 | С | | B2114 | 22.617 | | 21.106 | 1.00 16.39 | C |
| MOTA | 1786 | 0 | VAI | B2114 | 22.578 | | 20.492 | | 0 |
| ATOM | 1787 | N | ILI | E B2115 | 23.724 | | | | N |
| ATOM | 1788 | CA | IL | E B2115 | 25.014 | -1.093 | 20.763 | 1.00 15.53 | С |
| | | | | | | | | | |

| MOTA | 1789 | СВ | ILE : | B2115 | 25.589 | -0.191 | 19.664 | 1.00 16.8 | 2 | С |
|--------------|--------------|-----|-------|---------|------------------|-----------------|------------------|----------------------|----|--------|
| MOTA | 1790 | | | B2115 | 26.983 | -0.702 | 19.253 | 1.00 14.2 | 5 | С |
| MOTA | 1791 | | | B2115 | 24.649 | -0.168 | 18.461 | 1.00 17.2 | | С |
| ATOM | 1792 | | | B2115 | 25.020 | 0.874 | 17.423 | 1.00 18.6 | | С |
| ATOM | 1793 | С | ILE | B2115 | 25.956 | -1.039 | 21.956 | 1.00 16.8 | 8 | С |
| ATOM | 1794 | | | B2115 | 26.080 | 0.006 | 22.614 | 1.00 16.0 | 2 | 0 |
| ATOM | 1795 | | | B2116 | 26.603 | -2.164 | 22.237 | 1.00 14.9 | 8 | N |
| ATOM | 1796 | | | B2116 | 27.529 | -2.259 | 23.361 | 1.00 16.5 | | С |
| ATOM | 1797 | | | B2116 | 27.365 | -3.605 | 24.067 | 1.00 16.2 | | С |
| ATOM | 1798 | | LEU | B2116 | 25.945 | -3.870 | 24.578 | 1.00 16.4 | | С |
| ATOM | 1799 | | | B2116 | 25.872 | -5.256 | 25.197 | 1.00 15.7 | | С |
| ATOM | 1800 | CD2 | LEU | B2116 | 25.563 | -2.803 | 25.591 | 1.00 15.0 | | С |
| ATOM | 1801 | С | LEU | B2116 | 28.945 | -2.121 | 22.852 | 1.00 17.6 | | С |
| ATOM | 1802 | 0 | LEU | B2116 | 29.297 | -2.703 | 21.827 | 1.00 17.8 | 88 | 0 |
| MOTA | 1803 | N | GLU | B2117 | 29.763 | -1.373 | 23.584 | 1.00 19.1 | | N |
| ATOM | 1804 | CA | GLU | B2117 | 31.132 | -1.136 | 23.166 | 1.00 22.4 | 4 | С |
| ATOM | 1805 | CB | GLU | B2117 | 31.199 | 0.229 | 22.473 | 1.00 21.5 | | С |
| ATOM | 1806 | CG | GLU | B2117 | 32.570 | 0.672 | 22.003 | 1.00 26.0 | | С |
| ATOM | 1807 | CD | GLU | B2117 | 32.563 | 2.110 | 21.477 | 1.00 26.2 | | С |
| ATOM | 1808 | OE1 | GLU | B2117 | 31.958 | 2.997 | 22.132 | 1.00 24.1 | | 0 |
| ATOM | 1809 | OE2 | GLU | B2117 | 33.170 | 2.355 | 20.412 | 1.00 27.5 | | 0 |
| ATOM | 1810 | С | GLU | B2117 | 32.116 | -1.191 | 24.335 | 1.00 24.5 | | C |
| MOTA | 1811 | 0 | GLU | B2117 | 31.829 | -0.711 | 25.432 | 1.00 21.9 | | 0 |
| ATOM | 1812 | N | GLU | B2118 | 33.266 | -1.806 | 24.084 | 1.00 26.3 | | N |
| MOTA | 1813 | CA | GLU | B2118 | 34.331 | -1.920 | 25.070 | 1.00 31.0 | | C |
| MOTA | 1814 | CB | GLU | B2118 | 34.781 | -3.373 | 25.209 | 1.00 33.0 | | С |
| MOTA | 1815 | CG | GLU | B2118 | 33.888 | -4.220 | 26.082 | 1.00 38.0 | | C |
| ATOM | 1816 | CD | GLU | B2118 | 34.094 | -3.939 | 27.552 | 1.00 42. | | C |
| MOTA | 1817 | | | B2118 | 33.776 | -2.816 | 27.998 | 1.00 44. | | 0 |
| MOTA | 1818 | OE2 | GLU | B2118 | 34.584 | -4.845 | 28.262 | 1.00 45. | | 0 |
| MOTA | 1819 | С | | B2118 | 35.482 | -1.091 | 24.533 | 1.00 32. | | C |
| ATOM | 1820 | 0 | | B2118 | 35.880 | -0.108 | 25.197 | 1.00 35. | | 0 |
| MOTA | 1821 | OXT | | B2118 | 35.958 | -1.442 | 23.431 | 1.00 32. | 94 | 0 |
| TER | 1822 | | | B2118 | | | 10 001 | 1 00 30 | 22 | C |
| MOTA | 1823 | CB | | C3003 | 37.039 | 0.395 | 12.081 | 1.00 32. | | C C |
| MOTA | 1824 | CG | | C3003 | 37.297 | -0.447 | 10.845 | 1.00 36. | | s |
| MOTA | 1825 | SD | | C3003 | 38.483 | 0.306 | 9.716 | 1.00 46. | | C |
| MOTA | 1826 | CE | | C3003 | 37.454 | 1.490 | 8.876 | 1.00 42. | | C |
| ATOM | 1827 | С | | C3003 | 34.864 | -0.764 | 12.331 | 1.00 25. | | 0 |
| MOTA | 1828 | 0 | | C3003 | 34.821 | -1.903 | 11.864 | 1.00 26. 1.00 27. | | N |
| MOTA | 1829 | N | | C3003 | 36.772 | -1.388 | 13.778 | 1.00 27. | | C |
| MOTA | 1830 | CA | | C3003 | 36.090 | -0.264 | 13.082 12.219 | 1.00 27. | | N |
| MOTA | 1831 | Ŋ | | C3004 | 33.866 | 0.097 -0.247 | 11.500 | 1.00 23. | | C |
| ATOM | 1832 | CA | | C3004 | 32.655 | | 11.890 | 1.00 21. | | C |
| MOTA | 1833 | | | C3004 | 31.503 | 0.697 | 11.063 | 1.00 22. | | Č |
| MOTA | 1834 | | | C3004 | 30.259 | 0.377 | 13.391 | 1.00 20. | | Č |
| ATOM | 1835 | | | C3004 | 31.212 30.181 | 1:530 | 13.913 | 1.00 20. | | č |
| MOTA | 1836 | | | C3004 | 32.942 | -0.109 | 10.005 | 1.00 22. | | Ċ |
| MOTA | 1837 | C | | C3004 | 33.595 | 0.843 | 9.578 | 1.00 21. | | 0 |
| MOTA | 1838 | 0 | | C3004 | | -1.071 | 9.212 | 1.00 21. | | N |
| ATOM | 1839 | N | | C3005 | 32.483 32.692 | -0.999 | 7.777 | 1.00 22. | | C |
| MOTA | 1840 | CA | | . C3005 | 33.600 | -2.145 | 7.265 | 1.00 24 | | C |
| ATOM | 1841 | | | C3005 | 34.954 | -2.143 | 7.205 | | | C |
| ATOM | 1842 1843 | | | C3005 | 32.924 | -3.487 | 7.478 | | | C |
| ATOM ATOM | 1843 | | | C3005 | 31.349 | -1.036 | | | | C |
| | | | | C3005 | 31.297 | -0.988 | 5.823 | | | 0 |
| MOTA | 1845 | | AUT | - 65005 | 31.231 | 0.500 | | | | |

| 7.00 | 3046 | | CT 17 | 02006 | 20 064 | 1 100 | 7 014 | 1 00 10 77 | |
|------|------|-----|-------|-------|--------|--------|--------|------------|---|
| ATOM | 1846 | N | | C3006 | 30.264 | -1.106 | 7.814 | 1.00 19.77 | N |
| MOTA | 1847 | CA | GLY | C3006 | 28.946 | -1.124 | 7.207 | 1.00 18.90 | С |
| ATOM | 1848 | С | GLY | C3006 | 27.840 | -1.111 | 8.240 | 1.00 18.66 | С |
| ATOM | 1849 | 0 | GLY | C3006 | 28.039 | -1.542 | 9.375 | 1.00 19.40 | 0 |
| ATOM | 1850 | N | | C3007 | 26.679 | -0.595 | 7.849 | 1.00 17.60 | N |
| ATOM | 1851 | CA | | C3007 | 25.517 | -0.544 | 8.726 | 1.00 17.25 | Ċ |
| ATOM | 1852 | СВ | | C3007 | _ | 0.709 | 9.615 | | C |
| | | | | | 25.541 | | | 1.00 17.61 | |
| ATOM | 1853 | CG | | C3007 | 24.315 | 0.867 | 10.469 | 1.00 17.57 | С |
| ATOM | 1854 | | | C3007 | 23.615 | 1.967 | 10.834 | 1.00 17.24 | С |
| ATOM | 1855 | ND1 | HIS | C3007 | 23.686 | -0.203 | 11.072 | 1.00 17.16 | N |
| ATOM | 1856 | CE1 | HIS | C3007 | 22.651 | 0.231 | 11.771 | 1.00 17.81 | С |
| ATOM | 1857 | NE2 | HIS | C3007 | 22.585 | 1.545 | 11.644 | 1.00 18.60 | N |
| MOTA | 1858 | С | | C3007 | 24.264 | -0.540 | 7.867 | 1.00 17.20 | С |
| ATOM | 1859 | ō | | C3007 | 24.138 | 0.249 | 6.924 | 1.00 17.44 | Ö |
| | | | | | | | | | |
| ATOM | 1860 | N | | C3008 | 23.335 | -1.427 | 8.187 | 1.00 16.34 | N |
| ATOM | 1861 | CA | | C3008 | 22.111 | -1.484 | 7.416 | 1.00 18.39 | С |
| ATOM | 1862 | С | | C3008 | 20.925 | -1.924 | 8.242 | 1.00 19.04 | С |
| ATOM | 1863 | 0 | GLY | C3008 | 21.060 | -2.752 | 9.145 | 1.00 19.03 | 0 |
| ATOM | 1864 | И . | ILE | C3009 | 19.761 | -1.352 | 7.944 | 1.00 18.83 | N |
| MOTA | 1865 | CA | ILE | C3009 | 18.542 | -1.718 | 8.640 | 1.00 19.42 | С |
| ATOM | 1866 | CB | | C3009 | 18.047 | -0.598 | 9.594 | 1.00 18.51 | С |
| ATOM | 1867 | | | C3009 | 19.197 | -0.150 | 10.493 | 1.00 20.36 | č |
| ATOM | 1868 | | | C3009 | 17.505 | 0.585 | 8.797 | 1.00 17.23 | Č |
| | | | | | | | | | |
| ATOM | 1869 | | | C3009 | 16.778 | 1.592 | 9.643 | 1.00 13.66 | С |
| ATOM | 1870 | С | | C3009 | 17.473 | -1.992 | 7.602 | 1.00 18.70 | C |
| ATOM | 1871 | 0 | | C3009 | 17.647 | -1.685 | 6.427 | 1.00 15.95 | 0 |
| MOTA | 1872 | N | ASP | C3010 | 16.369 | -2.585 | 8.037 | 1.00 19.75 | N |
| MOTA | 1873 | CA | ASP | C3010 | 15.278 | -2.882 | 7.129 | 1.00 20.22 | C |
| MOTA | 1874 | CB | ASP | C3010 | 15.550 | -4.184 | 6.358 | 1.00 20.94 | С |
| MOTA | 1875 | CG | ASP | C3010 | 14.474 | -4.487 | 5.310 | 1.00 22.14 | С |
| MOTA | 1876 | | | C3010 | 14.480 | -3.844 | 4.236 | 1.00 22.44 | 0 |
| ATOM | 1877 | | | C3010 | 13.617 | -5.363 | 5.561 | 1.00 20.92 | Ö |
| ATOM | 1878 | C | | C3010 | 14.007 | -3.047 | 7.932 | 1.00 20.32 | c |
| | | | | | | | | | |
| ATOM | 1879 | 0 | | C3010 | 14.042 | -3.500 | 9.078 | 1.00 21.26 | 0 |
| ATOM | 1880 | N | | C3011 | 12.893 | -2.646 | 7.333 | 1.00 19.66 | N |
| ATOM | 1881 | CA | | C3011 | 11.588 | -2.813 | 7.949 | 1.00 20.09 | С |
| ATOM | 1882 | CB | | C3011 | 10.959 | -1.476 | 8.400 | 1.00 20.39 | C |
| ATOM | 1883 | CG2 | ILE | C3011 | 10.910 | -0.478 | 7.234 | 1.00 16.27 | C |
| ATOM | 1884 | CG1 | ILE | C3011 | 9.561 | -1.753 | 8.971 | 1.00 20.84 | С |
| ATOM | 1885 | CD1 | ILE | C3011 | 9.081 | -0.712 | 9.969 | 1.00 21.63 | С |
| ATOM | 1886 | С | ILE | C3011 | 10.777 | -3.440 | 6.825 | 1.00 21.21 | С |
| MOTA | 1887 | 0 | | C3011 | 10.866 | -3.006 | 5.678 | 1.00 21.49 | Ō |
| ATOM | 1888 | N | • | C3012 | 10.018 | -4.481 | 7.140 | 1.00 21.79 | N |
| ATOM | 1889 | CA | | C3012 | 9.249 | | 6.120 | | C |
| | | | | | | -5.174 | | 1.00 23.44 | |
| ATOM | 1890 | CB | | C3012 | 10.024 | -6.415 | 5.656 | 1.00 24.63 | c |
| MOTA | 1891 | CG | | C3012 | 9.269 | -7.309 | 4.667 | 1.00 27.74 | С |
| ATOM | 1892 | CD | | C3012 | 9.351 | -6.812 | 3.237 | 1.00 27.70 | С |
| ATOM | 1893 | OE1 | GLU | C3012 | 9.663 | -5:626 | 3.032 | 1.00 28.89 | 0 |
| ATOM | 1894 | OE2 | GLU | C3012 | 9.091 | -7.612 | 2.314 | 1.00 31.17 | 0 |
| ATOM | 1895 | С | GLU | C3012 | 7.873 | -5.583 | 6.625 | 1.00 23.57 | С |
| ATOM | 1896 | 0 | | C3012 | 7.750 | -6.258 | 7.647 | 1.00 22.12 | 0 |
| ATOM | 1897 | N | | C3013 | 6.840 | -5.170 | 5.904 | 1.00 23.45 | N |
| ATOM | 1898 | CA | | C3013 | 5.491 | | | | C |
| | | | | | | -5.519 | 6.286 | 1.00 24.76 | |
| ATOM | 1899 | CB | | C3013 | 4.479 | -4.613 | 5.571 | 1.00 29.22 | C |
| ATOM | 1900 | CG | | C3013 | 3.662 | -3.731 | 6.531 | 1.00 33.17 | C |
| ATOM | 1901 | CD | | C3013 | 3.915 | -2.242 | 6.349 | 1.00 38.85 | С |
| MOTA | 1902 | OE1 | GLU | C3013 | 3.660 | -1.719 | 5.238 | 1.00 44.44 | 0 |

| ATOM | 1903 | OF2 | GLII | C3013 | 4.359 | -1.586 | 7.318 | 1.00 3 | 0 04 | 0 |
|------|------|-----|------|-------|-------|--------------------|--------|-----------|------|---|
| ATOM | 1904 | C | | C3013 | | | | | | 0 |
| ATOM | 1904 | | | | 5.238 | -6.993 | 5.963 | 1.00 2 | | C |
| | | 0 | | C3013 | 5.643 | -7.502 | 4.910 | 1.00 2 | | 0 |
| ATOM | 1906 | N | | C3014 | 4.599 | -7.685 | 6.898 | 1.00 2 | | N |
| MOTA | 1907 | CA | | C3014 | 4.287 | -9.092 | 6.712 | 1.00 2 | | С |
| MOTA | 1908 | CB | | C3014 | 3.531 | -9.613 | 7.939 | 1.00 2 | 8.12 | С |
| ATOM | 1909 | CG | | C3014 | 4.251 | -10.630 | 8.829 | 1.00 3 | 1.98 | C |
| ATOM | 1910 | | | C3014 | 5.647 | -10.144 | 9.191 | 1.00 3 | 1.03 | С |
| ATOM | 1911 | CD2 | LEU | C3014 | 3.414 | -10.868 | 10.083 | 1.00 3 | 3.69 | C |
| ATOM | 1912 | С | LEU | C3014 | 3.453 | -9.308 | 5.439 | 1.00 2 | 5.44 | C |
| ATOM | 1913 | 0 | LEU | C3014 | 3.554 | -10.345 | 4.793 | 1.00 2 | 5.78 | 0 |
| ATOM | 1914 | N | ALA | C3015 | 2.644 | -8.320 | 5.073 | 1.00 2 | 4.83 | N |
| ATOM | 1915 | CA | ALA | C3015 | 1.801 | -8.438 | 3.879 | 1.00 2 | 7.12 | С |
| MOTA | 1916 | CB | ALA | C3015 | 0.915 | -7.206 | 3.747 | 1.00 2 | | Č |
| ATOM | 1917 | С | ALA | C3015 | 2.592 | -8.659 | 2.584 | 1.00 2 | | Č |
| ATOM | 1918 | 0 | | C3015 | 2.215 | -9.497 | 1.761 | 1.00 2 | | Ö |
| ATOM | 1919 | N | | C3016 | 3.683 | -7.916 | 2.399 | 1.00 2 | | N |
| ATOM | 1920 | CA | | C3016 | 4.498 | -8.062 | 1.192 | 1.00 2 | | c |
| ATOM | 1921 | СВ | | C3016 | 5.706 | -7.117 | 1.232 | 1.00 2 | | C |
| ATOM | 1922 | OG | | C3016 | 5.324 | -5.799 | 1.573 | 1.00 2 | | 0 |
| ATOM | 1923 | c | | C3016 | 4.997 | -9.502 | 1.072 | 1.00 2 | | C |
| ATOM | 1924 | Ō | | C3016 | | -10.062 | -0.027 | 1.00 2 | | |
| ATOM | 1925 | N | | C3017 | | -10.094 | 2.212 | 1.00 2 | | 0 |
| ATOM | 1926 | CA | | C3017 | | | | | | N |
| ATOM | 1927 | CB | | C3017 | | -11.464 -11.771 | 2.248 | 1.00 2 | | C |
| ATOM | | • | | | | | 3.613 | 1.00 2 | | C |
| | 1928 | CG2 | | C3017 | | -13.241 | 3.688 | 1.00 2 | | C |
| ATOM | 1929 | | | C3017 | | -10.863 | 3.808 | 1.00 2 | | С |
| ATOM | 1930 | | | C3017 | | -11.007 | 2.735 | 1.00 2 | | С |
| ATOM | 1931 | C | | C3017 | | -12.456 | 2.019 | 1.00 2 | | С |
| ATOM | 1932 | 0 | | C3017 | | -13.408 | 1.253 | 1.00 2 | | 0 |
| ATOM | 1933 | N | | C3018 | | -12.235 | 2.690 | 1.00 2 | | N |
| MOTA | 1934 | CA | | C3018 | | -13.122 | 2.534 | 1.00 2 | | С |
| ATOM | 1935 | CB | | C3018 | | -12.645 | 3.427 | 1.00 2 | | С |
| ATOM | 1936 | CG | | C3018 | | -12.504 | 4.884 | 1.00 3 | 2.78 | С |
| MOTA | 1937 | CD | | C3018 | | -11.783 | 5.722 | 1.00 3 | 4.19 | С |
| MOTA | 1938 | OE1 | | C3018 | | -10.865 | 5.190 | 1.00 3 | 4.18 | 0 |
| ATOM | 1939 | | | C3018 | | -12.118 | 6.920 | 1.00 3 | 5.99 | 0 |
| MOTA | 1940 | С | GLU | C3018 | 1.983 | -13.163 | 1.067 | 1.00 2 | 9.36 | С |
| MOTA | 1941 | 0 | | C3018 | 1.763 | -14.239 | 0.507 | 1.00 2 | 8.97 | 0 |
| ATOM | 1942 | N | SER | C3019 | 1.867 | -11.994 | 0.440 | 1.00 2 | 8.95 | N |
| ATOM | 1943 | CA | SER | C3019 | 1.454 | -11.931 | -0.957 | 1.00 2 | 9.90 | C |
| ATOM | 1944 | CB | SER | C3019 | 1.285 | -10.476 | -1.410 | 1.00 3 | 0.07 | С |
| ATOM | 1945 | OG | SER | C3019 | 2.542 | -9.866 | -1.632 | 1.00 3 | 3.15 | 0 |
| ATOM | 1946 | C | SER | C3019 | 2.489 | -12.623 | -1.837 | 1.00 3 | 0.43 | С |
| ATOM | 1947 | 0 | SER | C3019 | 2.138 | -13.362 | -2.755 | 1.00 3 | 0.07 | 0 |
| ATOM | 1948 | N | ALA | C3020 | 3.766 | -12.391 | -1.549 | 1.00 2 | 9.14 | N |
| ATOM | 1949 | CA | ALA | C3020 | 4.842 | -12.994 | -2.327 | 1.00 3 | | C |
| ATOM | 1950 | CB | ALA | C3020 | | -12:465 | -1.847 | 1.00 3 | | С |
| ATOM | 1951 | С | ALA | C3020 | 4.834 | -14.527 | -2.269 | 1.00 3 | | C |
| ATOM | 1952 | 0 | ALA | C3020 | | -15.198 | -3.264 | 1.00 3 | | 0 |
| MOTA | 1953 | N | | C3021 | | -15.082 | -1.103 | 1.00 3 | | N |
| MOTA | 1954 | CA | | C3021 | | -16.532 | -0.959 | 1.00 3 | | C |
| ATOM | 1955 | CB | | C3021 | | -16.950 | 0.489 | 1.00 3 | | Ċ |
| ATOM | 1956 | | | C3021 | | -18.465 | 0.565 | 1.00 3 | | Č |
| MOTA | 1957 | | | C3021 | | -16.521 | 1.414 | 1.00 3 | | C |
| ATOM | 1958 | С | | C3021 | | -17.135 | -1.896 | 1.00 3 | | č |
| ATOM | 1959 | Ō | | C3021 | | -18.094 | -2.616 | 1.00 3 | | Ö |
| | | | | | 950 | | | ~ · · · · | | |

| ATOM | 1960 | N | THR | C3022 | 2.263 | -16.552 | -1.889 | 1.00 36. | 26 | N |
|------|------|-----|-----|--------|--------|---------|--------|----------|----|---|
| ATOM | 1961 | CA | THR | C3022 | 1.166 | -17.019 | -2.726 | 1.00 38. | | С |
| MOTA | 1962 | CB | THR | C3022 | -0.142 | -16.274 | -2.371 | 1.00 38. | 89 | С |
| ATOM | 1963 | OG1 | THR | C3022 | -0.532 | -16.613 | -1.034 | 1.00 39. | 61 | 0 |
| MOTA | 1964 | CG2 | THR | C3022 | -1.262 | -16.654 | -3.336 | 1.00 37. | 67 | С |
| ATOM | 1965 | С | THR | C3022 | 1.458 | -16.836 | -4.214 | 1.00 40. | 67 | С |
| ATOM | 1966 | 0 | THR | C3022 | 1.325 | -17.772 | -5.005 | 1.00 40. | | 0 |
| MOTA | 1967 | N | | C3023 | | -15.626 | -4.587 | 1.00 42. | | N |
| ATOM | 1968 | CA | | C3023 | | -15.303 | -5.974 | 1.00 46. | | C |
| ATOM | 1969 | СВ | | C3023 | | -13.944 | -6.037 | 1.00 46. | | Ċ |
| ATOM | 1970 | CG | | C3023 | | -13.278 | -7.396 | 1.00 47. | | č |
| ATOM | 1971 | CD | | C3023 | | -11.827 | -7.269 | 1.00 47. | | č |
| ATOM | 1972 | NE | | C3023 | | -11.695 | -6.577 | 1.00 48. | | N |
| ATOM | 1973 | CZ | | C3023 | | -10.924 | -5.511 | 1.00 48. | | C |
| ATOM | 1974 | | | C3023 | | -10.214 | -5.008 | 1.00 46. | | N |
| ATOM | 1975 | | | C3023 | | -10.861 | -4.948 | 1.00 48. | | N |
| ATOM | 1976 | С | | C3023 | | -16.391 | -6.616 | 1.00 47. | | C |
| ATOM | 1977 | Ō | | C3023 | | -16.906 | -7.681 | 1.00 49. | | ő |
| ATOM | 1978 | N | | C3024 | | -16.737 | -5.968 | 1.00 49. | | N |
| ATOM | 1979 | CA | | C3024 | | -17.787 | -6.458 | 1.00 50. | | C |
| ATOM | 1980 | СВ | | C3024 | | -17.193 | -7.045 | 1.00 51. | | C |
| ATOM | 1981 | CG | | C3024 | | -16.464 | -8.338 | 1.00 53. | | c |
| ATOM | 1982 | | | C3024 | | -16.754 | -9.597 | 1.00 53. | | C |
| ATOM | 1983 | | | C3024 | | -15.282 | -8.426 | 1.00 54. | | Ŋ |
| ATOM | 1984 | | | C3024 | | -14.875 | -9.683 | 1.00 54. | | C |
| ATOM | 1985 | | | C3024 | | -15.750 | | 1.00 53. | | N |
| ATOM | 1986 | C | | C3024 | | -18.720 | -5.304 | 1.00 50. | | C |
| ATOM | 1987 | 0 | | C3024 | | -18.314 | -4.347 | 1.00 50. | | 0 |
| ATOM | 1988 | N | | C3025 | | -19.971 | -5.394 | 1.00 30. | | И |
| ATOM | 1989 | CA | | C3025 | | -20.937 | -4.335 | 1.00 49. | | C |
| ATOM | 1990 | CB | | C3025 | | -22.270 | -4.632 | 1.00 49. | | C |
| ATOM | 1991 | CG | | C3025 | | -23.331 | -3.575 | 1.00 55. | | C |
| ATOM | 1992 | CD | | C3025 | | -24.694 | -3.972 | 1.00 57. | | C |
| ATOM | 1993 | | | C3025 | | -24.870 | -4.053 | 1.00 57. | | 0 |
| ATOM | 1994 | | | C3025 | | -25.590 | -4.206 | 1.00 59. | | 0 |
| ATOM | 1995 | C | | C3025 | | -21.182 | -4.118 | 1.00 46. | | C |
| ATOM | 1996 | 0 | | C3025 | | -21.711 | -3.084 | 1.00 47. | | 0 |
| ATOM | 1997 | N | | C3025 | | -20.801 | -5.092 | 1.00 47. | | N |
| ATOM | 1998 | CA | | C3026 | | -20.997 | -4.956 | 1.00 44. | | C |
| ATOM | 1999 | C | | C3026 | | -19.811 | -4.320 | | | c |
| ATOM | 2000 | 0 | | C3026 | | -19.768 | -4.265 | 1.00 40. | | 0 |
| ATOM | 2001 | N | | C3027 | | -18.842 | -3.841 | 1.00 37. | | N |
| ATOM | 2002 | CA | | C3027 | | -17.655 | -3.217 | 1.00 37. | | C |
| ATOM | 2002 | CB | | C3027 | | -16.715 | -2.738 | 1.00 33. | | C |
| ATOM | 2004 | CG | | .C3027 | | | | 1.00 34. | | c |
| ATOM | 2005 | | | C3027 | | -14.569 | -2.700 | 1.00 33. | | c |
| MOTA | 2006 | | | C3027 | | -15.277 | -0.687 | 1.00 33. | | c |
| ATOM | 2007 | | | C3027 | | -13.450 | -2.042 | 1.00 32. | | c |
| ATOM | 2008 | | | C3027 | | -14.163 | -0.016 | 1.00 32. | | C |
| ATOM | 2009 | CZ | | C3027 | | -13.248 | -0.696 | 1.00 33. | | C |
| ATOM | 2010 | C | | C3027 | | -13.246 | -2.042 | 1.00 33. | | C |
| ATOM | 2010 | 0 | | C3027 | | -17.688 | -2.042 | 1.00 34. | | 0 |
| ATOM | 2012 | N | | C3028 | | -17.088 | -1.071 | 1.00 34. | | N |
| ATOM | 2012 | CA | | C3028 | | -19.159 | 0.109 | 1.00 33. | | C |
| ATOM | 2013 | CB | | C3028 | | -19.159 | 0.109 | 1.00 34. | | C |
| ATOM | 2015 | C | | C3028 | | -19.885 | -0.263 | 1.00 33. | | C |
| ATOM | 2016 | 0 | | C3028 | | -19.572 | 0.257 | 1.00 34. | | 0 |
| | 2010 | ~ | 1 | 00020 | 12.073 | 17.512 | 0.237 | 1.00 54. | | O |

| ATOM · | 2017 | N | LYS | C3029 | 11.683 | -20.854 | -1.166 | 1.00 33.7 | 3 N |
|--------|------|-----|-----|-------|--------|---------|---------|-----------|-----|
| ATOM | 2018 | CA | LYS | C3029 | 12.831 | -21.636 | -1.605 | 1.00 32.8 | 7 C |
| ATOM | 2019 | CB | LYS | C3029 | 12.396 | -22.671 | -2.650 | 1.00 32.2 | В С |
| MOTA | 2020 | CĢ | LYS | C3029 | 11.313 | -23.617 | -2.157 | 0.05 32.4 | О С |
| MOTA | 2021 | CD | LYS | C3029 | 10.821 | -24.537 | -3.261 | 0.05 32.2 | В С |
| ATOM | 2022 | CE | LYS | C3029 | 9.721 | -25.456 | -2.753 | 0.05 32.2 | 0 с |
| MOTA | 2023 | NZ | LYS | C3029 | 9.160 | -26.313 | -3.833 | 0.05 32.1 | 5 ท |
| MOTA | 2024 | С | LYS | C3029 | 13.910 | -20.735 | -2.181 | 1.00 32.7 | о с |
| MOTA | 2025 | 0 | LYS | C3029 | 15.100 | -21.016 | -2.048 | 1.00 33.4 | 4 0 |
| ATOM | 2026 | N | ARG | C3030 | 13.498 | -19.643 | -2.814 | 1.00 32.8 | 5 ท |
| ATOM | 2027 | CA | ARG | C3030 | 14.458 | -18.714 | -3.397 | 1.00 32.5 | 3 с |
| ATOM | 2028 | CB | ARG | C3030 | 13.796 | -17.877 | -4.497 | 0.05 32.5 | |
| MOTA | 2029 | CG | | C3030 | 13.442 | -18.670 | -5.747 | 0.05 32.7 | |
| ATOM | 2030 | CD | | C3030 | 13.135 | -17.752 | -6.922 | 0.05 32.8 | |
| ATOM | 2031 | NE | | C3030 | | -16.973 | -6.722 | 0.05 33.0 | |
| ATOM | 2032 | CZ | | C3030 | | -17.490 | -6.720 | 0.05 33.1 | |
| ATOM | 2033 | NH1 | | C3030 | | -18.791 | -6.908 | 0.05 33.1 | |
| ATOM | 2034 | | | C3030 | | -16.705 | -6.531 | 0.05 33.0 | |
| ATOM | 2035 | С | | C3030 | | -17.794 | -2.351 | 1.00 32.3 | |
| ATOM | 2036 | 0 | | C3030 | | -17.408 | -2.470 | 1.00 32.8 | |
| ATOM | 2037 | N | | C3031 | | -17.455 | -1.325 | 1.00 31.5 | |
| ATOM | 2038 | CA | | C3031 | | -16.574 | -0.245 | 1.00 30.1 | |
| ATOM | 2039 | СВ | | C3031 | | -15.905 | 0.469 | 1.00 30.4 | |
| ATOM | 2040 | | | C3031 | | -15.140 | 1.701 | 1.00 31.9 | |
| ATOM | 2041 | | | C3031 | | -14.967 | -0.484 | 1.00 31.3 | |
| ATOM | 2042 | С | | C3031 | | -17.284 | 0.836 | 1.00 29.7 | |
| ATOM | 2043 | Ō | | C3031 | | -16.686 | 1.439 | 1.00 29.4 | |
| ATOM | 2044 | N | | C3032 | | -18.554 | 1.076 | 1.00 27.3 | |
| MOTA | 2045 | CA | | C3032 | | -19.338 | . 2.119 | 1.00 25.9 | |
| ATOM | 2046 | СВ | | C3032 | | -19.917 | 3.047 | 1.00 24.7 | |
| ATOM | 2047 | CG | | C3032 | | -18.943 | 3.572 | 1.00 22.8 | |
| ATOM | 2048 | | | C3032 | | -19.708 | 4.361 | 1.00 23.1 | |
| ATOM | 2049 | | | C3032 | | -17.893 | 4.452 | 1.00 21.5 | |
| ATOM | 2050 | C | | C3032 | | -20.485 | 1.630 | 1.00 27.2 | |
| ATOM | 2051 | Ö | | C3032 | | -21.187 | 0.676 | 1.00 28.3 | |
| ATOM | 2052 | N | | C3033 | | -20.676 | 2.307 | 1.00 26.4 | |
| ATOM | 2053 | CA | | C3033 | | -21.756 | 1.984 | 1.00 27.3 | |
| MOTA | 2054 | CB | | C3033 | | -21.662 | 2.795 | 1.00 25.6 | |
| ATOM | 2055 | OG1 | | C3033 | | -21.820 | 4.186 | 1.00 26.3 | |
| ATOM | 2056 | | | C3033 | | -20.323 | 2.574 | 1.00 26.7 | |
| ATOM | 2057 | С | | C3033 | | -23.062 | 2.385 | 1.00 27.7 | |
| ATOM | 2058 | 0 | THR | C3033 | | -23.061 | 2.920 | 1.00 28.1 | |
| MOTA | 2059 | N | | C3034 | | -24.174 | 2.145 | 1.00 28.9 | |
| MOTA | 2060 | CA | | C3034 | | -25.484 | 2.493 | 1.00 29.0 | |
| ATOM | 2061 | СВ | | C3034 | 19.283 | -26.572 | | 1.00 29.4 | |
| ATOM | 2062 | С | ALA | C3034 | | -25.594 | 3.990 | 1.00 28.6 | |
| ATOM | 2063 | 0 | | C3034 | | -26.008 | 4.403 | 1.00 29.5 | |
| ATOM | 2064 | N | | C3035 | | -25:218 | 4.805 | 1.00 28.0 | |
| ATOM | 2065 | CA | LEU | C3035 | | -25.310 | 6.249 | 1.00 27.6 | |
| ATOM | 2066 | СВ | | C3035 | | -24.964 | 6.952 | 1.00 29.3 | |
| ATOM | 2067 | CG | | C3035 | | -25.809 | 8.190 | 1.00 31.5 | |
| ATOM | 2068 | | | C3035 | | -27.297 | 7.821 | 1.00 32.2 | |
| ATOM | 2069 | CD2 | LEU | C3035 | | -25.438 | 8.727 | 1.00 30.0 | |
| ATOM | 2070 | С | | C3035 | 17.740 | -24.410 | 6.747 | 1.00 27.5 | |
| ATOM | 2071 | 0 | LEU | C3035 | | -24.832 | 7.571 | 1.00 26.2 | |
| ATOM | 2072 | N | | C3036 | 17.688 | -23.176 | 6.247 | 1.00 27.3 | |
| ATOM | 2073 | CA | | C3036 | 16.636 | -22.240 | 6.649 | 1.00 27.2 | |

| ATOM | 2074 | СВ | GLU | C3036 | 16.849 | -20.877 | 5.981 | 1.00 25.56 | 5 C |
|------|------|------|-----|-------|--------|-----------|--------|------------|------------|
| ATOM | 2075 | CG | GLU | C3036 | 17.834 | -19.978 | 6.707 | 1.00 22.65 | S C |
| MOTA | 2076 | CD . | GLU | C3036 | 18.256 | -18.777 | 5.880 | 1.00 23.21 | C |
| MOTA | 2077 | OE1 | GLU | C3036 | 18.735 | -17.784 | 6.469 | 1.00 22.56 | 5 0 |
| ATOM | 2078 | OE2 | GLU | C3036 | 18.124 | -18.825 | 4.638 | 1.00 24.80 |) 0 |
| ATOM | 2079 | С | | C3036 | 15.258 | -22.793 | 6.278 | 1.00 28.00 | С С |
| ATOM | 2080 | 0 | GLU | C3036 | 14.306 | -22.668 | 7.047 | 1.00 27.30 |) 0 |
| ATOM | 2081 | N | MET | C3037 | 15.160 | -23.401 | 5.098 | 1.00 28.24 | l N |
| ATOM | 2082 | CA | MET | C3037 | 13.897 | -23.979 | 4.641 | 1.00 30.24 | l C |
| ATOM | 2083 | CB | MET | C3037 | 14.051 | -24.593 | 3.247 | 1.00 31.74 | l C |
| ATOM | 2084 | CG | MET | C3037 | 13.885 | -23.605 | 2.102 | 1.00 32.50 | 5 C |
| ATOM | 2085 | SD | MET | C3037 | 12.289 | -22.761 | 2.156 | 1.00 37.45 | 5 S |
| ATOM | 2086 | CE | MET | C3037 | 11.153 | -24.108 | 1.753 | 1.00 36.0 | 7 C |
| ATOM | 2087 | С | MET | C3037 | 13.411 | -25.049 | 5.608 | 1.00 31.10 | 5 C |
| MOTA | 2088 | 0 | MET | C3037 | 12.222 | -25.124 | 5.920 | 1.00 30.59 | 5 0 |
| MOTA | 2089 | N | GLU | C3038 | 14.336 | -25.882 | 6.076 | 1.00 31.23 | N N |
| ATOM | 2090 | CA | GLU | C3038 | 13.992 | -26.936 | 7.018 | 1.00 31.3 | 5 C |
| MOTA | 2091 | CB | GLU | C3038 | | -27.635 | 7.525 | 0.05 30.99 | 5 C |
| ATOM | 2092 | CG | GLU | C3038 | 15.478 | -29.023 | 6.948 | 0.05 30.58 | 3 C |
| ATOM | 2093 | CD | GLU | C3038 | 16.721 | -29.692 | 7.504 | 0.05 30.43 | l C |
| ATOM | 2094 | OE1 | GLU | C3038 | 16.840 | -29.795 | 8.744 | 0.05 30.03 | 3 0 |
| ATOM | 2095 | OE2 | GLU | C3038 | 17.578 | -30.118 | 6.702 | 0.05 30.19 | 5 0 |
| MOTA | 2096 | С | GLU | C3038 | 13.235 | -26.330 | 8.191 | 1.00 31.5 | 3 C |
| ATOM | 2097 | 0 | GLU | C3038 | 12.255 | -26.897 | 8.663 | 1.00 32.13 | 5 0 |
| ATOM | 2098 | N | ARG | C3039 | 13.697 | -25.176 | 8.664 | 1.00 32.0 | N C |
| MOTA | 2099 | CA | ARG | C3039 | 13.046 | -24.496 | 9.781 | 1.00 33.2 | 1 C |
| MOTA | 2100 | СВ | ARG | C3039 | 13.928 | -23.353 | 10.289 | 1.00 34.1 | 1 C |
| ATOM | 2101 | CG | ARG | C3039 | 13.317 | -22.548 | 11.434 | 1.00 37.6 | 8 C |
| ATOM | 2102 | CD | ARG | C3039 | 13.189 | -23.377 | 12.704 | 1.00 39.5 | 9 C |
| ATOM | 2103 | NE | ARG | C3039 | 12.565 | -22.626 | 13.791 | 1.00 41.9 | 2 N |
| ATOM | 2104 | CZ | ARG | C3039 | 12.195 | -23.159 | 14.952 | 1.00 43.0 | 2 C |
| ATOM | 2105 | NH1 | ARG | C3039 | 12.384 | -24.450 | 15.183 | 1.00 43.5 | |
| ATOM | 2106 | NH2 | ARG | C3039 | 11.625 | -22.402 | 15.881 | 1.00 44.0 | 0 N |
| ATOM | 2107 | С | ARG | C3039 | 11.692 | -23.939 | 9.339 | 1.00 32.7 | 0 C |
| ATOM | 2108 | 0 | ARG | C3039 | 10.674 | -24.130 | 10.005 | 1.00 31.8 | 1 0 |
| ATOM | 2109 | N | PHE | C3040 | 11.699 | -23.240 | 8.210 | 1.00 32.8 | |
| MOTA | 2110 | CA | PHE | C3040 | 10.489 | -22.646 | 7.653 | 1.00 33.5 | |
| ATOM | 2111 | CB | | C3040 | 10.778 | -22.128 | 6.242 | 1.00 32.0 | |
| MOTA | 2112 | CG | PHE | C3040 | | -21.604 | 5.528 | 1.00 32.5 | |
| MOTA | 2113 | | | C3040 | 9.012 | -20.380 | 5.880 | 1.00 31.2 | |
| MOTA | 2114 | | | C3040 | 8.980 | -22.340 | 4.503 | 1.00 32.7 | |
| MOTA | 2115 | | | C3040 | | -19.895 | 5.222 | 1.00 31.9 | |
| ATOM | 2116 | | | C3040 | | -21.865 | 3.839 | 1.00 33.2 | |
| MOTA | 2117 | CZ | PHE | C3040 | 7.301 | -20.637 | 4.201 | 1.00 31.4 | |
| MOTA | 2118 | С | | C3040 | | -23.680 | 7.595 | | |
| MOTA | 2119 | 0 | | C3040 | | -23.457 | 8.100 | 1.00 33.3 | |
| MOTA | 2120 | N | | C3041 | | -24.819 | 6.983 | 1.00 34.6 | |
| MOTA | 2121 | CA | | C3041 | | -25.898 | 6.828 | 1.00 35.5 | |
| MOTA | 2122 | CB | | C3041 | | -27.002 | 5.923 | 1.00 36.2 | |
| ATOM | 2123 | | | C3041 | | -26.464 | 4.616 | 1.00 38.0 | |
| MOTA | 2124 | | | C3041 | | -28.170 | 5.813 | 1.00 36.6 | |
| MOTA | 2125 | С | | C3041 | | -26.517 | 8.143 | 1.00 36.0 | |
| MOTA | 2126 | 0 | | C3041 | | -26.945 | 8.247 | 1.00 37.2 | |
| ATOM | 2127 | N | | C3042 | | -26.560 | 9.147 | 1.00 36.6 | |
| MOTA | 2128 | CA | | C3042 | | -27.142 | 10.427 | 1.00 37.3 | |
| MOTA | 2129 | CB | | C3042 | | 2 -27.377 | 11.303 | 1.00 38.4 | |
| ATOM | 2130 | OG | SER | C3042 | 10.391 | -26.172 | 11.904 | 1.00 39.3 | 1 0 |

| ATOM | 2131 | С | SER | C3042 | 7.744 | -26.230 | 11.157 | 1.00 37.81 | | С |
|--------|------|-----|---------|-------|--------|---------|--------|------------|---|---|
| ATOM | 2132 | 0 | SER | C3042 | 7.010 | -26.671 | 12.042 | 1.00 38.07 | | 0 |
| ATOM | 2133 | | | C3043 | 7.740 | -24.956 | 10.781 | 1.00 37.43 | | N |
| ATOM | 2134 | | | C3043 | | -23.969 | 11.400 | 1.00 37.02 | | С |
| ATOM | 2135 | | | C3043 | | -22.600 | 11.428 | 1.00 37.05 | | С |
| | | | | C3043 | | -22.327 | 12.513 | 1.00 37.93 | | Č |
| ATOM | 2136 | | | | | | • | | | C |
| ATOM | 2137 | | | C3043 | | -23.470 | 12.628 | 1.00 39.39 | | |
| ATOM | 2138 | | | C3043 | | -21.040 | 12.177 | 1.00 38.02 | | C |
| ATOM | 2139 | | | C3043 | | -23.851 | 10.666 | 1.00 37.04 | | С |
| MOTA | 2140 | 0 | LEU | C3043 | 5.389 | -24.291 | 9.522 | 1.00 37.65 | | 0 |
| ATOM | 2141 | N | LYS | C3044 | 4.542 | -23.250 | 11.325 | 1.00 36.12 | | N |
| ATOM | 2142 | CA | LYS | C3044 | 3.236 | -23.075 | 10.707 | 1.00 35.63 | | С |
| ATOM | 2143 | CB | LYS | C3044 | 2.313 | -24.246 | 11.072 | 1.00 37.63 | | С |
| ATOM | 2144 | CG | | C3044 | | -24.356 | 12.555 | 1.00 40.09 | | C |
| ATOM | 2145 | | | C3044 | | -25.432 | 12.813 | 1.00 42.38 | | С |
| ATOM | 2146 | CE | | C3044 | | -26.813 | 12.365 | 1.00 42.85 | | č |
| | | | | | | -27.847 | 12.550 | 1.00 43.11 | | N |
| ATOM | 2147 | NZ | | C3044 | | | | 1.00 33.57 | | C |
| ATOM | 2148 | C | | C3044 | | -21.753 | 11.111 | | | |
| ATOM | 2149 | 0 | | C3044 | | -21.116 | 12.086 | 1.00 33.02 | • | 0 |
| ATOM | 2150 | N | | C3045 | | -21.345 | 10.339 | 1.00 31.64 | | N |
| ATOM | 2151 | CA | | C3045 | | -20.115 | 10.618 | 1.00 29.90 | | С |
| ATOM | 2152 | C · | GLY | C3045 | 1.689 | -18.844 | 10.666 | 1.00 28.38 | | С |
| ATOM | 2153 | 0 | GLY | C3045 | 2.643 | -18.676 | 9.915 | 1.00 28.13 | | 0 |
| ATOM | 2154 | N | ARG | C3046 | 1.299 | -17.946 | 11.564 | 1.00 28.66 | | N |
| ATOM | 2155 | CA | ARG | C3046 | 1.957 | -16.661 | 11.758 | 1.00 27.23 | | С |
| ATOM | 2156 | CB | ARG | C3046 | 1.279 | -15.920 | 12.912 | 0.05 27.45 | | С |
| ATOM | 2157 | CG | | C3046 | -0.235 | -15.860 | 12.769 | 0.05 27.80 | | С |
| ATOM | 2158 | CD | | C3046 | | -15.403 | 14.048 | 0.05,28.08 | | С |
| ATOM | 2159 | NE | | C3046 | | -15.526 | 13.962 | 0.05 28.35 | | N |
| | | | | | | -15.249 | 14.959 | 0.05 28.51 | | C |
| ATOM | 2160 | CZ | | C3046 | | | | 0.05 28.59 | | N |
| ATOM | 2161 | | | C3046 | | -15.394 | 14.792 | | | N |
| MOTA | 2162 | | | C3046 | | -14.831 | 16.127 | 0.05 28.63 | | |
| MOTA | 2163 | С | | C3046 | | -16.827 | 12.041 | 1.00 26.66 | | C |
| MOTA | 2164 | 0 | | C3046 | | -16.065 | 11.537 | 1.00 23.83 | | 0 |
| ATOM | 2165 | N | | C3047 | | -17.824 | 12.847 | 1.00 26.74 | | N |
| ATOM | 2166 | CA | ARG | C3047 | 5.197 | -18.068 | 13.172 | 1.00 28.45 | | С |
| MOTA | 2167 | CB | ARG | C3047 | 5.330 | -19.223 | 14.167 | 1.00 30.78 | | С |
| MOTA | 2168 | CG | ARG | C3047 | 4.824 | -18.919 | 15.567 | 1.00 36.74 | | С |
| MOTA | 2169 | CD | ARG | C3047 | 5.548 | -19.793 | 16.580 | 1.00 40.75 | | С |
| ATOM | 2170 | NE | ARG | C3047 | 6.991 | -19.561 | 16.540 | 1.00 43.99 | | N |
| ATOM | 2171 | CZ | | C3047 | | -20.341 | 17.126 | 1.00 45.84 | | C |
| ATOM | 2172 | | | C3047 | • | -21.417 | 17.803 | 1.00 47.05 | | N |
| ATOM | 2173 | | | C3047 | | -20.046 | 17.036 | 1.00 46.26 | , | N |
| ATOM | 2174 | C | | C3047 | | -18.396 | 11.924 | 1.00 26.96 | | C |
| | 2175 | | | C3047 | | -18.019 | | 1.00 27.18 | | ō |
| ATOM | | | | | | | 10.989 | 1.00 27.16 | | N |
| ATOM | 2176 | N | | C3048 | | -19.108 | | 1.00 23.10 | | C |
| ATOM | 2177 | CA | | C3048 | | -19.474 | 9.765 | | | C |
| MOTA | 2178 | CB | | C3048 | | -20.489 | 8.964 | 1.00 24.71 | | |
| MOTA | 2179 | CG | | C3048 | | -21.176 | 7.884 | 1.00 24.87 | | C |
| MOTA | 2180 | CD | | C3048 | | -22.028 | 6.947 | 1.00 27.10 | | C |
| MOTA | 2181 | | | C3048 | | -23.007 | 6.393 | 1.00 28.27 | | 0 |
| ATOM | 2182 | NE2 | GLN | C3048 | 4.000 | -21.650 | 6.747 | 1.00 27.28 | | N |
| MOTA | 2183 | С | GLN | C3048 | 6.342 | -18.240 | 8.907 | 1.00 23.81 | | С |
| ATOM | 2184 | 0 | | C3048 | 7.441 | -18.064 | 8.376 | 1.00 22.00 | ı | 0 |
| ATOM | 2185 | N | | C3049 | | -17.394 | 8.767 | 1.00 23.83 | | N |
| ATOM | 2186 | CA | | C3049 | | -16.174 | 7.972 | 1.00 22.84 | | С |
| ATOM | 2187 | СВ | | C3049 | | -15.428 | 7.889 | 1.00 23.39 | | Ċ |
| AT OFF | 2101 | CD | ندند .د | 00043 | 3.093 | 13.720 | | 1.00 20.00 | | _ |

| ATOM | 2188 | CG2 | ILE | C3049 | 4.270 | -14.110 | 7.123 | 1.00 20.78 | С |
|--------------|--------------|-----------|-----|----------------|--------|--------------------|------------------|--------------------------|--------|
| ATOM | 2189 | CG1 | ILE | C3049 | 3.068 | -16.317 | 7.194 | 1.00 25.01 | C |
| ATOM | 2190 | CD1 | ILE | C3049 | 1.637 | -15.812 | 7.313 | 1.00 28.28 | C |
| ATOM | 2191 | С | ILE | C3049 | 6.492 | -15.254 | 8.596 | 1.00 22.76 | С |
| ATOM | 2192 | 0 | ILE | C3049 | 7.334 | -14.695 | 7.901 | 1.00 22.64 | 0 |
| ATOM | 2193 | N | GLU | C3050 | 6.426 | -15.119 | 9.917 | 1.00 23.06 | N |
| MOTA | 2194 | CA | GLU | C3050 | 7.347 | -14.287 | 10.685 | 1.00 23.40 | С |
| MOTA | 2195 | CB | GLU | C3050 | 7.023 | -14.436 | 12.169 | 1.00 27.99 | С |
| ATOM | 2196 | CG | GLU | C3050 | | -13.229 | 13.014 | 1.00 34.34 | С |
| ATOM | 2197 | CD | | C3050 | | -11.997 | 12.501 | 1.00 37.30 | С |
| ATOM | 2198 | | | C3050 | • | -11.233 | 11.752 | 1.00 38.54 | 0 |
| MOTA | 2199 | | | C3050 | | -11.807 | 12.825 | 1.00 38.13 | 0 |
| ATOM | 2200 | С | | C3050 | | -14.707 | 10.429 | 1.00 22.91 | С |
| ATOM | 2201 | 0 | | C3050 | | -13.863 | 10.212 | 1.00 19.78 | O N |
| ATOM | 2202 | N | | C3051 | | -16.018 | 10.451 | 1.00 20.98 | C |
| ATOM | 2203 | CA | | C3051 | | -16.549 | 10.218 10.286 | 1.00 20.98 | C |
| ATOM | 2204 | CB | | C3051 | | -18.087 -18.710 | 9.996 | 1.00 20.94 | c |
| ATOM | 2205 | CG CD1 | | C3051 | | -19.072 | 8.699 | 1.00 21.88 | C |
| ATOM ATOM | 2206 2207 | | | C3051 | | -19.563 | 8.420 | 1.00 22.08 | Č |
| ATOM | 2207 | | | C3051 | | -18.864 | 11.011 | 1.00 24.22 | Č |
| ATOM | 2209 | | | C3051 | | -19.353 | 10.743 | 1.00 22.50 | Ċ |
| ATOM | 2210 | CZ | | C3051 | | -19.695 | 9.447 | 1.00 23.28 | С |
| ATOM | 2211 | OH | | C3051 | | -20.142 | 9.181 | 1.00 26.17 | 0 |
| ATOM | 2212 | C. | | C3051 | | -16.093 | 8.863 | 1.00 21.41 | C |
| MOTA | 2213 | 0 | | C3051 | | -15.508 | 8.764 | 1.00 20.67 | 0 |
| ATOM | 2214 | N | | C3052 | | -16.357 | 7.823 | 1.00 20.18 | N |
| ATOM | 2215 | CA | | C3052 | | -15.985 | 6.465 | 1.00 19.73 | С |
| ATOM | 2216 | CB | | C3052 | | -16.399 | 5.502 | 1.00 20.90 | С |
| ATOM | 2217 | CG | LEU | C3052 | 9.488 | -16.052 | 4.019 | 1.00 20.73 | С |
| MOTA | 2218 | CD1 | LEU | C3052 | 10.837 | -16.537 | 3.484 | 1.00 21.92 | C |
| ATOM | 2219 | CD2 | LEU | C3052 | 8.329 | -16.704 | 3.247 | 1.00 22.34 | C |
| MOTA | 2220 | С | LEU | C3052 | 10.725 | -14.487 | 6.365 | 1.00 18.62 | С |
| MOTA | 2221 | 0 | LEU | C3052 | 11.745 | -14.057 | 5.819 | 1.00 18.97 | 0 |
| MOTA | 2222 | N | ALA | C3053 | | -13.697 | 6.912 | 1.00 18.23 | N |
| MOTA | 2223 | CA | ALA | C3053 | | -12.238 | 6.888 | 1.00 19.28 | C |
| MOTA | 2224 | CB | | C3053 | | -11.611 | 7.489 | 1.00 19.78 | C |
| ATOM | 2225 | С | | C3053 | | -11.746 | 7.634 | 1.00 18.63 | С |
| ATOM | 2226 | 0 | | C3053 | | -10.815 | 7.191 | 1.00 17.69 | O N |
| ATOM | 2227 | N | | C3054 | | -12.375 | 8.767 | 1.00 18.30 | C |
| ATOM | 2228 | CA | | C3054 | | -11.989 -12.303 | 9.534 8.776 | 1.00 18.14 1.00 19.55 | C |
| ATOM | 2229 | C | | C3054 C3054 | | -12.505 | 8.831 | 1.00 19.33 | ő |
| ATOM | 2230 2231 | O N | | C3054 | | -13.421 | 8.060 | 1.00 18.30 | N |
| ATOM ATOM | 2231 | CA | | C3055 | | -13.783 | | 1.00 19.48 | Ċ |
| ATOM | 2232 | CB | | C3055 | | -15.239 | 6.839 | 1.00 20.53 | c |
| ATOM | 2234 | CG | | C3055 | | -16.213 | 7.709 | 1.00 22.48 | С |
| ATOM | 2235 | CD | | C3055 | | -16:093 | 9.181 | 1.00 26.13 | С |
| ATOM | 2236 | NE | | C3055 | | -16.945 | 10.019 | 1.00 28.05 | N |
| ATOM | 2237 | CZ | | C3055 | | -16.972 | 11.347 | 1.00 28.02 | С |
| ATOM | 2238 | | | C3055 | | -16.190 | 11.999 | 1.00 28.89 | N |
| ATOM | 2239 | | | C3055 | | -17.788 | 12.024 | 1.00 28.23 | N |
| ATOM | 2240 | С | | C3055 | | -12.849 | 6.108 | 1.00 20.40 | С |
| ATOM | 2241 | 0 | | C3055 | | -12.399 | 5.817 | 1.00 20.36 | 0 |
| ATOM | 2242 | N | | C3056 | 14.182 | -12.547 | 5, 424 | 1.00 20.72 | N |
| MOTA | 2243 | CA | TRE | C3056 | | -11.641 | 4.280 | 1.00 22.18 | С |
| MOTA | 2244 | CB | TRE | C3056 | 12.837 | -11.486 | 3.655 | 1.00 23.99 | С |
| | | | | | | | | | |

| ATOM | 2245 | CG | TRP | C3056 | 12.716 | -10.303 | 2.719 | 1.00 29.31 | . С |
|--------------|----------------------|----------|-----|----------------|--------|--------------------|----------------|------------|-----|
| ATOM | 2246 | CD2 | TRP | C3056 | 12.723 | -10.335 | 1.289 | 1.00 30.25 | C |
| MOTA | 2247 | CE2 | TRP | C3056 | 12.609 | -9.001 | 0.840 | 1.00 32.03 | C C |
| ATOM | 2248 | CE3 | TRP | C3056 | 12.821 | -11.362 | 0.342 | 1.00 33.18 | |
| ATOM | 2249 | CD1 | TRP | C3056 | 12.598 | -8.984 | 3.070 | 1.00 30.82 | |
| ATOM | 2250 | NE1 | | C3056 | 12.532 | | 1.947 | 1.00 33.62 | |
| MOTA | 2251 | | | C3056 | 12.582 | | -0.515 | 1.00 34.74 | |
| ATOM | 2252 | | | C3056 | 12.795 | -11.029 | -1.010 | 1.00 34.82 | |
| MOTA | 2253 | | | C3056 | 12.679 | | -1.425 | 1.00 36.26 | |
| MOTA | 2254 | С | | C3056 | | -10.284 | 4.760 | 1.00 20.86 | |
| MOTA | 2255 | 0 | | C3056 | 15.608 | | 4.134 | 1.00 18.98 | |
| ATOM | 2256 | N | | C3057 | 14.206 | | 5.885 | 1.00 18.95 | |
| ATOM | 2257 | CA | | C3057 | 14.586 | | 6.487 | 1.00 19.90 | |
| MOTA | 2258 | CB | | C3057 | 13.755 | | 7.752 | 1.00 21.78 | |
| MOTA | 2259 | OG | | C3057 | 14.067 | | 8.342 | 1.00 25.39 | |
| ATOM | 2260 | С | | C3057 | 16.070 | | 6.841 | 1.00 18.84 | |
| ATOM | 2261 | 0 | | C3057 | 16.767 | | 6.514 | 1.00 19.51 | |
| MOTA | 2262 | N | | C3058 | 16.550 | | 7.509 | 1.00 18.85 | |
| ATOM | 2263 | CA | | C3058 | 17.949 | | 7.917 | 1.00 18.94 | |
| ATOM | 2264 | СВ | | C3058 | | -10.854 | 8.765 | 1.00 16.80 | |
| ATOM | 2265 | C | | C3058 | 18.912 | | 6.730 | 1.00 19.28 | |
| ATOM | 2266 | 0 | | C3058 | 19.955 | | 6.765 | 1.00 19.4 | |
| ATOM | 2267 | N | | C3059 C3059 | | -10.349 -10.432 | 5.683 4.507 | 1.00 18.93 | |
| ATOM | 2268 | CA | | | | | 3.604 | 1.00 19.00 | |
| ATOM | 2269 | CB CG | | C3059 | | -11.575 -12.925 | 4.271 | 1.00 20.1 | |
| ATOM ATOM | 2270 2 271 | CD | | C3059 | | -14.069 | 3.331 | 1.00 17.40 | |
| ATOM | 2272 | CE | | C3059 | | -15.392 | 4.070 | 1.00 21.3 | |
| | 2273 | NZ | | C3059 | | -16.545 | 3.158 | 1.00 24.9 | |
| ATOM | 2274 | C | | C3059 | 19.437 | | 3.744 | 1.00 21.3 | |
| ATOM ATOM | 2275 | 0 | | C3059 | 20.457 | | 3.165 | 1.00 21.3 | |
| ATOM | 2276 | N | | C3060 | 18.297 | | 3.745 | 1.00 22.2 | |
| ATOM | 2277 | CA | | C3060 | 18.175 | | 3.080 | 1.00 22.2 | |
| ATOM | 2278 | CB | | C3060 | 16.708 | | 3.076 | 1.00 24.9 | |
| ATOM | 2279 | CG | | C3060 | 16.424 | | 2.373 | 1.00 32.6 | |
| ATOM | 2280 | CD | | C3060 | 16.807 | | 0.901 | 1.00 37.1 | |
| ATOM | 2281 | | | C3060 | 16.401 | | | 1.00 38.3 | |
| ATOM | 2282 | | | C3060 | 17.509 | | 0.456 | 1.00 38.7 | |
| MOTA | 2283 | С | | C3060 | 19.042 | | 3.864 | 1.00 20.9 | 4 C |
| MOTA | 2284 | 0 | GLU | C3060 | 19.829 | -5.429 | 3.285 | 1.00 22.9 | 3 0 |
| MOTA | 2285 | N | ALA | C3061 | 18.907 | -6.178 | 5.186 | 1.00 19.6 | 8 N |
| ATOM | 2286 | CA | ALA | C3061 | 19.698 | -5.282 | 6.024 | 1.00 20.1 | |
| ATOM | 2287 | CB | ALA | C3061 | 19.373 | -5.515 | 7.499 | 1.00 19.4 | |
| ATOM | 2288 | С | ALA | C3061 | 21.185 | -5.520 | 5.759 | 1.00 19.1 | 4 C |
| ATOM | 2289 | 0 | ALA | C3061 | 21.953 | -4.576 | 5.572 | 1.00 18.8 | |
| MOTA | 2290 | N | PHE | C3062 | 21.588 | | 5.723 | 1.00 19.9 | |
| MOTA | 2291 | CA | | C3062 | 22.987 | | 5.465 | 1.00 19.7 | |
| ATOM | 2292 | CB | | C3062 | 23.214 | | 5.570 | 1.00 20.8 | |
| ATOM | 2293 | CG | | C3062 | 24.604 | | 5.171 | 1.00 21.1 | |
| ATOM | 2294 | | | C3062 | 24.896 | | 3.847 | 1.00 21.2 | |
| ATOM | 2295 | | | C3062 | 25.629 | | 6.109 | 1.00 20.4 | |
| ATOM | 2296 | | | C3062 | 26.195 | | 3.463 | 1.00 22.3 | |
| ATOM | 2297 | | | C3062 | 26.930 | | 5.738 | 1.00 21.9 | |
| MOTA | 2298 | CZ | | C3062 | 27.211 | | 4.410 | 1.00 22.0 | |
| ATOM | 2299 | С | | C3062 | 23.443 | | 4.089 | 1,00 21.3 | |
| ATOM | 2300 | 0 | | C3062 | 24.526 | | 3.951 | 1.00 20.7 | |
| ATOM | 2301 | N | 251 | C3063 | 22.612 | 2 -6.843 | 3.074 | 1.00 22.1 | 7 N |

| ATOM | 2302 | CA | SER | C3063 | 22.949 | -6.434 | 1.717 | 1.00 22.74 | С |
|------|------|-----|-----|-------|--------|---------|------------------|------------|----|
| ATOM | 2303 | CB | SER | C3063 | 21.851 | -6.873 | 0.754 | 1.00 23.43 | С |
| MOTA | 2304 | OG | SER | C3063 | 21.635 | -8.265 | 0.877 | 1.00 28.48 | 0 |
| MOTA | 2305 | С | SER | C3063 | 23.123 | -4.926 | 1.649 | 1.00 22.84 | С |
| ATOM | 2306 | 0 | | C3063 | 24.001 | -4.422 | 0.947 | 1.00 21.58 | 0 |
| ATOM | 2307 | | | C3064 | 22.277 | -4.205 | 2.377 | 1.00 21.35 | N |
| ATOM | 2308 | CA | | C3064 | 22.370 | -2.755 | 2.406 | 1.00 21.55 | Ċ |
| | 2309 | CB | | C3064 | 21.111 | -2.168 | 3.055 | 1.00 22.13 | c |
| ATOM | | | | | | | 2.238 | 1.00 22.13 | C |
| ATOM | 2310 | CG | | C3064 | 19.841 | -2.416 | | 1.00 21.86 | |
| ATOM | 2311 | CD | | C3064 | 18.588 | -1.884 | 2.929 | | С |
| ATOM | 2312 | CE | | C3064 | 18.653 | -0.375 | 3.120 | 1.00 22.07 | C |
| MOTA | 2313 | NZ | | C3064 | 17.579 | 0.125 | 4.017 | 1.00 21.49 | N |
| MOTA | 2314 | С | | C3064 | 23.639 | -2.341 | 3.168 | 1.00 21.95 | С |
| MOTA | 2315 | 0 | | C3064 | 24.295 | -1.363 | 2.812 | 1.00 22.05 | 0 |
| MOTA | 2316 | N | ALA | C3065 | 23.994 | -3.104 | 4.197 | 1.00 20.93 | N |
| MOTA | 2317 | CA | ALA | C3065 | 25.193 | -2.818 | 4.983 | 1.00 23.70 | С |
| ATOM | 2318 | CB | ALA | C3065 | 25.254 | -3.729 | 6.200 | 1.00 22.08 | C |
| ATOM | 2319 | C | ALA | C3065 | 26.450 | -3.010 | 4.136 | 1.00 25.75 | С |
| ATOM | 2320 | 0 | ALA | C3065 | 27.420 | -2.278 | 4.297 | 1.00 25.29 | 0 |
| MOTA | 2321 | N | | C3066 | 26.433 | -4.008 | 3.255 | 1.00 27.80 | N |
| ATOM | 2322 | CA | | C3066 | 27.569 | -4.278 | 2.375 | 1.00 31.06 | С |
| ATOM | 2323 | СВ | | C3066 | 27.386 | -5.616 | 1.649 | 1.00 30.03 | С |
| ATOM | 2324 | CG | | C3066 | 27.666 | -6.848 | 2.495 | 1.00 30.77 | č |
| | 2325 | SD | | C3066 | 29.395 | -6.944 | 3.059 | 1.00 31.09 | S |
| ATOM | | | | | | | | | C |
| ATOM | 2326 | CE | | C3066 | 30.192 | -7.610 | 1.576 | 1.00 29.01 | |
| MOTA | 2327 | С | | C3066 | 27.683 | -3.159 | 1.342 | 1.00 33.44 | С |
| ATOM | 2328 | 0 | | C3066 | 28.778 | -2.782 | 0.940 | 1.00 32.94 | O. |
| ATOM | 2329 | N | | C3067 | 26.539 | | 0.918 | 1.00 36.57 | N |
| ATOM | 2330 | CA | | C3067 | 26.542 | | -0.059 | 1.00 40.47 | C |
| MOTA | 2331 | С | | C3067 | 26.101 | | -1.426 | 1.00 43.36 | С |
| ATOM | 2332 | 0 | GLY | C3067 | 26.602 | | -2.447 | 1.00 44.87 | 0 |
| MOTA | 2333 | N | THR | C3068 | 25.161 | | -1.447 | 0.05 44.27 | N |
| MOTA | 2334 | CA | THR | C3068 | 24.650 | -3.506 | -2.701 | 0.05 45.40 | С |
| MOTA | 2335 | CB | THR | C3068 | 25.521 | -4.680 | -3.201 | 0.05 45.40 | С |
| ATOM | 2336 | OG1 | THR | C3068 | 25.018 | -5.147 | -4.459 | 0.05 45.48 | 0 |
| ATOM | 2337 | CG2 | THR | C3068 | 25.518 | -5.821 | -2.193 | 0.05 45.43 | С |
| ATOM | 2338 | С | THR | C3068 | 23.212 | -3.973 | -2.507 | 0.05 46.15 | С |
| ATOM | 2339 | 0 | THR | C3068 | 22.452 | -3.355 | -1.761 | 0.05 46.24 | 0 |
| ATOM | 2340 | N | GLY | C3069 | 22.839 | -5.058 | -3.175 | 0.05 47.05 | N |
| ATOM | 2341 | CA | | C3069 | 21.488 | | -3.043 | 0.05 48.19 | С |
| ATOM | 2342 | С | | C3069 | 21.341 | | -3.555 | 0.05 48.95 | С |
| ATOM | 2343 | Ō | | C3069 | 22.322 | | -3.927 | 0.05 49.00 | 0 |
| ATOM | 2344 | N | | C3070 | 20.106 | | -3.569 | 0.05 49.77 | N |
| ATOM | 2345 | CA | | C3070 | 19.809 | | -4.038 | 0.05 50.58 | C |
| ATOM | 2346 | CB | | C3070 | 18.311 | | -3.800 | 0.05 50.80 | Č |
| ATOM | 2347 | | | C3070 | 17.434 | | -4.584 | 0.05 51.01 | Ċ |
| ATOM | 2348 | | | C3070 | | -10.600 | -4.205 | 0.05 51.05 | c |
| | | | | C3070 | | -11:631 | -3.486 | 0.05 51.19 | C |
| ATOM | 2349 | | | | | | | 0.05 50.91 | Ċ |
| ATOM | 2350 | С | | C3070 | 20.140 | | -5.528 -6.126 | 0.05 50.91 | 0 |
| ATOM | 2351 | 0 | | C3070 | 20.642 | | -6.126 | | N |
| ATOM | 2352 | N | | C3071 | | -10.093 | -6.108 | 0.05 51.31 | |
| ATOM | 2353 | CA | | C3071 | | -10.372 | -7.522 | 0.05 51.63 | C |
| ATOM | 2354 | CB | | C3071 | 19.393 | | -8.411 | 0.05 51.73 | С |
| MOTA | 2355 | OG | | C3071 | 20.018 | | -8.363 | 0.05 51.85 | 0 |
| MOTA | 2356 | C | | C3071 | | -10.420 | -7.891 | 0.05 51.76 | C |
| ATOM | 2357 | 0 | | C3071 | | -11.053 | -8.878 | 0.05 51.87 | 0 |
| MOTA | 2358 | N | LYS | C3072 | 22.433 | -9.755 | -7.106 | 0.05 51.86 | N |
| | | | | | | | | | |

| ATOM | 2359 | CA | LYS | C3072 | 23.867 | -9.751 | -7.374 | 0.05 5 | 1.85 | C | |
|------|------|-----|-----|-------|--------|-----------|--------|--------|-------|---|---|
| ATOM | 2360 | CB | LYS | C3072 | 24.396 | -8.312 | -7.449 | 0.05 5 | 2.23 | C | : |
| ATOM | 2361 | CG | LYS | C3072 | 24.392 | -7.543 | -6.131 | 0.05 5 | 2.70 | C | ; |
| ATOM | 2362 | CD | LYS | C3072 | 25.580 | -7.907 | -5.245 | 0.05 5 | 3.07 | C | |
| MOTA | 2363 | CE | LYS | C3072 | 26.905 | -7.581 | -5.920 | 0.05 5 | 3.33 | C | ; |
| ATOM | 2364 | NZ | LYS | C3072 | 27.022 | -6.134 | -6.253 | 0.05 5 | 3.48 | ħ | Ŋ |
| ATOM | 2365 | С | LYS | C3072 | 24.606 | -10.529 | -6.292 | 0.05 5 | 1.55 | C | 7 |
| ATOM | 2366 | 0 | LYS | C3072 | 25.643 | -11.140 | -6.550 | 0.05 5 | 1.64 | C |) |
| ATOM | 2367 | N | LEU | C3073 | 24.062 | -10.500 | -5.080 | 0.05 5 | 1.11 | 7 | 1 |
| ATOM | 2368 | CA | LEU | C3073 | 24.660 | -11.204 | -3.953 | 0.05 5 | 0.57 | C | 2 |
| ATOM | 2369 | CB | LEU | C3073 | 24.615 | -10.328 | -2.699 | 0.05 5 | | | 3 |
| MOTA | 2370 | CG | LEU | C3073 | 25.349 | -10.863 | -1.467 | 0.05 5 | 0.92 | (| 2 |
| MOTA | 2371 | CD1 | LEU | C3073 | 26.830 | -11.010 | -1.783 | 0.05 5 | 1.03 | | 2 |
| ATOM | 2372 | CD2 | LEU | C3073 | 25.145 | -9.917 | -0.294 | 0.05 5 | 0.94 | (| 2 |
| MOTA | 2373 | С | LEU | C3073 | 23.893 | -12.498 | -3.707 | 0.05 5 | 0.00 | (| 2 |
| ATOM | 2374 | 0 | LEU | C3073 | 24.444 | -13.473 | -3.198 | 0.05 5 | 0.02 | (|) |
| MOTA | 2375 | N | GLY | C3074 | 22.616 | -12.492 | -4.076 | 1.00 4 | 9.38 | t | N |
| ATOM | 2376 | CA | GLY | C3074 | 21.779 | -13.663 | -3.899 | 1.00 4 | 8.02 | (| 0 |
| ATOM | 2377 | С | GLY | C3074 | 21.479 | -13.986 | -2.447 | 1.00 4 | 6.92 | (| C |
| ATOM | 2378 | 0 | GLY | C3074 | 22.391 | -14.150 | -1.642 | 1.00 4 | 6.73 | (| С |
| ATOM | 2379 | N | PHE | C3075 | | -14.076 | -2.107 | 1.00 4 | 6.04 | 1 | N |
| MOTA | 2380 | CA | | C3075 | 19.804 | -14.393 | -0.741 | 1.00 4 | 5.56 | (| С |
| MOTA | 2381 | СВ | | C3075 | | -14.137 | -0.544 | 1.00 4 | 5.22 | | С |
| ATOM | 2382 | CG | | C3075 | | -12.705 | -0.211 | 1.00 4 | 4.58 | | С |
| ATOM | 2383 | | | C3075 | | -11.724 | -0.187 | 1.00 4 | 4.91 | | С |
| ATOM | 2384 | | | C3075 | | -12.337 | 0.082 | 1.00 4 | | (| С |
| ATOM | 2385 | | | C3075 | | -10.397 | 0.127 | 1.00 4 | | | С |
| ATOM | 2386 | | | C3075 | | -11.016 | 0.398 | 1.00 4 | | | С |
| ATOM | 2387 | CZ | | C3075 | | -10.042 | 0.420 | 1.00 4 | | | С |
| ATOM | 2388 | C | | C3075 | | -15.841 | -0.407 | 1.00 4 | | | C |
| ATOM | 2389 | Õ | | C3075 | _ | -16.251 | 0.754 | 1.00 4 | | | Ō |
| ATOM | 2390 | N | | C3076 | | -16.607 | -1.433 | 1.00 4 | |] | N |
| ATOM | 2391 | CA | | C3076 | | -18.006 | -1.256 | 1.00 4 | | | С |
| ATOM | 2392 | CB | | C3076 | | -18.749 | -2.589 | 1.00 4 | | | С |
| ATOM | 2393 | CG | | C3076 | | -19.192 | -2.890 | 1.00 4 | | | С |
| ATOM | 2394 | CD | • | C3076 | | -20.206 | -1.880 | 1.00 4 | | | С |
| ATOM | 2395 | | | C3076 | | -20.367 | -1.676 | 1.00 4 | | | 0 |
| ATOM | 2396 | | | C3076 | | -20,906 | -1.245 | 1.00 4 | | | N |
| ATOM | 2397 | C | | C3076 | | -18.133 | -0.706 | 1.00 4 | | | С |
| ATOM | 2398 | Ö | | C3076 | | -19.165 | -0.149 | 1.00 4 | | | 0 |
| ATOM | 2399 | N | | C3077 | | -17.074 | -0.862 | 1.00 4 | | | N |
| ATOM | 2400 | CA | | C3077 | | -17.065 | -0.377 | 1.00 4 | 1.11 | | С |
| ATOM | 2401 | СВ | | C3077 | | -16.254 | -1.333 | 1.00 4 | 4.24 | | С |
| ATOM | 2402 | CG | | C3077 | | -16.789 | -2.756 | 1.00 4 | 15.88 | | С |
| ATOM | 2403 | OD1 | | C3077 | | -17.943 | -2.974 | 1.00 4 | | | 0 |
| MOTA | 2404 | | | C3077 | | -16.064 | -3.652 | 1.00 4 | | | 0 |
| ATOM | 2405 | С | | C3077 | | -16.481 | 1.028 | 1.00 3 | 38.51 | | С |
| ATOM | 2406 | 0 | | C3077 | | -16:291 | 1.598 | 1.00 3 | 39.35 | | 0 |
| ATOM | 2407 | N | | C3078 | | -16.194 | 1.578 | 1.00 | | i | N |
| ATOM | 2408 | CA | | C3078 | | -15.649 | 2.927 | 1.00 3 | | | С |
| ATOM | 2409 | CB | | C3078 | | -14.296 | 2.889 | 1.00 | 30.66 | | С |
| ATOM | 2410 | CG | | C3078 | | -13.026 | 2.584 | 1.00 | | | С |
| ATOM | 2411 | | | C3078 | | 3 -13.251 | 1.440 | 1.00 | | | С |
| ATOM | 2412 | | | C3078 | | 3 -11.900 | 2.254 | 1.00 | | | С |
| ATOM | 2413 | C | | C3078 | | -16.632 | 3.778 | 1.00 | | | С |
| ATOM | 2414 | Ö | | C3078 | | -17.178 | 3.322 | 1.00 | | | 0 |
| ATOM | 2415 | N | | C3079 | | -16.860 | 5.009 | 1.00 | | | N |
| | | | | | | | | | | | |

| MOTA | 2416 | CA | GLU | C3079 | 22.138 | -17.779 | 5.895 | 1.00 24.35 | С |
|------|------|---------|-----|-------|--------|--------------------|--------|--------------|---|
| ATOM | 2417 | CB | GLU | C3079 | 22.794 | -19.163 | 5.869 | 1.00 24.49 | С |
| ATOM | 2418 | CG | GLU | C3079 | 21.999 | -20.224 | 6.616 | 1.00 24.73 | C |
| MOTA | 2419 | CD | GLU | C3079 | 22.653 | -21.592 | 6.558 | 1.00 26.90 | С |
| ATOM | 2420 | | GLU | C3079 | 23.770 | -21.740 | 7.089 | 1.00 28.68 | 0 |
| ATOM | 2421 | | | C3079 | 22.053 | | 5.979 | 1.00 29.27 | 0 |
| ATOM | 2422 | | | C3079 | 22.098 | | 7.327 | 1.00 22.68 . | С |
| ATOM | 2423 | | | C3079 | 23.123 | | 7.883 | 1.00 22.88 | 0 |
| ATOM | 2424 | | | C3080 | 20.901 | | 7.907 | 1.00 21.79 | N |
| | 2425 | | | C3080 | 20.678 | | 9.276 | 1.00 21.18 | C |
| ATOM | 2425 | | | C3080 | 19.705 | | 9.325 | 1.00 22.20 | Č |
| ATOM | | | | C3080 | 19.404 | | 10.777 | 1.00 20.66 | c |
| MOTA | 2427 | | | C3080 | 20.311 | | 8.587 | 1.00 23.11 | c |
| ATOM | 2428 | | | | | | 10.060 | 1.00 20.45 | Č |
| ATOM | 2429 | | | C3080 | | -17.971 -18.429 | 9.743 | 1.00 20.45 | Ö |
| ATOM | 2430 | | | C3080 | | | | 1.00 19.30 | N |
| ATOM | 2431 | N ~~ | | C3081 | | -18.441 | 11.072 | | C |
| MOTA | 2432 | | | C3081 | | -19.540 | 11.897 | 1.00 21.15 | |
| ATOM | 2433 | CB | | C3081 | | -20.686 | 11.905 | 1.00 21.34 | C |
| MOTA | 2434 | CG | | C3081 | | -21.275 | 10.528 | 1.00 22.27 | C |
| ATOM | 2435 | | | C3081 | | -22.396 | 10.653 | 1.00 23.04 | C |
| MOTA | 2436 | CD2 | LEU | C3081 | | -21.802 | 9.884 | 1.00 24.47 | C |
| MOTA | 2437 | С | LEU | C3081 | | -19.003 | 13.300 | 1.00 21.01 | C |
| MOTA | 2438 | 0 | LEU | C3081 | | -17.811 | 13.541 | 1.00 20.54 | 0 |
| MOTA | 2439 | N | ASN | C3082 | 19.732 | -19.881 | 14.220 | 1.00 21.50 | N |
| ATOM | 2440 | CA | ASN | C3082 | 19.530 | -19.494 | 15.608 | 1.00 22.77 | С |
| MOTA | 2441 | CB | ASN | C3082 | | -19.783 | 16.020 | 1.00 23.53 | С |
| ATOM | 2442 | CG | ASN | C3082 | 17.099 | -18.880 | 15.310 | 1.00 25.44 | С |
| ATOM | 2443 | OD1 | ASN | C3082 | 16.907 | -17.731 | 15.698 | 1.00 25.60 | 0 |
| MOTA | 2444 | ND2 | ASN | C3082 | 16.488 | -19.388 | 14.247 | 1.00 27.37 | N |
| MOTA | 2445 | С | ASN | C3082 | 20.499 | -20.258 | 16.499 | 1.00 22.68 | С |
| ATOM | 2446 | 0 | ASN | C3082 | 20.629 | -21.478 | 16.380 | 1.00 21.84 | 0 |
| MOTA | 2447 | N | ASN | C3083 | 21.191 | -19.541 | 17.382 | 1.00 23.99 | N |
| ATOM | 2448 | CA | | C3083 | | -20.187 | 18.282 | 1.00 23.34 | С |
| MOTA | 2449 | СВ | | C3083 | 23.141 | -19.170 | 18.840 | 1.00 24.83 | С |
| MOTA | 2450 | CG | | C3083 | | -18.019 | 19.575 | 1.00 25.31 | С |
| ATOM | 2451 | | | C3083 | | -18.175 | 20.174 | 1.00 23.71 | 0 |
| ATOM | 2452 | | | C3083 | | -16.859 | 19.550 | 1.00 26.83 | N |
| ATOM | 2453 | C | | C3083 | | -20.877 | 19.415 | 1.00 25.05 | С |
| ATOM | 2454 | Õ | | C3083 | | -20.876 | 19.432 | 1.00 22.22 | 0 |
| ATOM | 2455 | N | | C3084 | | -21.460 | 20.365 | 1.00 27.04 | N |
| ATOM | 2456 | CA | | C3084 | | -22.174 | 21.466 | 1.00 29.78 | С |
| ATOM | 2457 | CB | | C3084 | | -22.954 | 22.275 | 1.00 32.58 | С |
| ATOM | 2458 | CG | | C3084 | | -22.141 | 22.711 | 1.00 36.99 | С |
| ATOM | 2459 | CD | | C3084 | | -22.184 | 21.707 | 1.00 41.57 | С |
| | 2460 | | | C3084 | • | -21.812 | 20.529 | 1.00 42.03 | 0 |
| ATOM | | | | C3084 | | -22.590 | 22.107 | 1.00 43.80 | 0 |
| ATOM | 2461 | | | C3084 | | -21.294 | 22.396 | 1.00 30.13 | Ċ |
| MOTA | 2462 | C | | | | | 23.111 | 1.00 30.13 | Ö |
| MOTA | 2463 | 0 | | C3084 | | -21:796 | | 1.00 30.37 | N |
| ATOM | 2464 | N | | C3085 | | -19.991 | 22.401 | 1.00 20.38 | C |
| ATOM | 2465 | CA | | C3085 | | -19.088 | 23.238 | | c |
| ATOM | 2466 | CB | | C3085 | | -17.912 | 23.716 | 1.00 31.17 | C |
| MOTA | 2467 | CG | | C3085 | | -18.340 | 24.705 | 1.00 34.80 | C |
| ATOM | 2468 | CD | | C3085 | | -17.237 | 24.995 | 1.00 37.35 | |
| MOTA | 2469 | NE | | C3085 | | -17.801 | 25.310 | 1.00 40.35 | N |
| MOTA | 2470 | CZ | | C3085 | | -18.518 | 26.396 | 1.00 40.77 | C |
| MOTA | 2471 | | | C3085 | | -18.757 | 27.285 | 1.00 42.29 | N |
| MOTA | 2472 | NH2 | ARG | C3085 | 25.852 | -19.007 | 26.587 | 1.00 41.71 | N |
| | | | | | | | | | |

| MOTA | 2473 | С | ARG | C3085 | | -18.597 | 22.438 | 1.00 29.32 | С |
|-------|------|-----|-----|-------|--------|-----------|--------|--------------------------|----------|
| MOTA | 2474 | 0 | ARG | C3085 | 18.112 | -17.806 | 22.923 | 1.00 30.16 | 0 |
| MOTA | 2475 | N | GLY | C3086 | 18.805 | -19.086 | 21.207 | 1.00 27.92 | N |
| ATOM | 2476 | CA | GLY | C3086 | 17.690 | -18.714 | 20.350 | 1.00 26.11 | C |
| ATOM | 2477 | С | GLY | C3086 | 17.893 | -17.452 | 19.530 | 1.00 25.66 | C |
| ATOM | 2478 | 0 | GLY | C3086 | 17.005 | -17.044 | 18.782 | 1.00 26.33 | 0 |
| ATOM | 2479 | N | ALA | C3087 | 19.061 | -16.831 | 19.654 | 1.00 23.88 | N |
| ATOM | 2480 | CA | ALA | C3087 | 19.328 | -15.613 | 18.914 | 1.00 22.63 | C |
| MOTA | 2481 | CB | ALA | C3087 | 20.408 | -14.797 | 19.610 | 1.00 21.67 | C |
| ATOM | 2482 | С | ALA | C3087 | 19.742 | -15.893 | 17.478 | 1.00 22.49 | С |
| ATOM | 2483 | 0 | ALA | C3087 | 20.515 | -16.808 | 17.210 | 1.00 22.63 | 0 |
| ATOM | 2484 | N | PRO | C3088 | 19.220 | -15.098 | 16.532 | 1.00 21.73 | N |
| MOTA | 2485 | CD | PRO | C3088 | | -14.068 | 16.740 | 1.00 21.19 | C |
| ATOM | 2486 | CA | PRO | C3088 | 19.536 | -15.244 | 15.112 | 1.00 20.08 | C |
| MOTA | 2487 | CB | PRO | C3088 | 18.434 | -14.435 | 14.435 | 1.00 22.01 | С |
| MOTA | 2488 | CG | PRO | C3088 | 18.196 | -13.325 | 15.412 | 1.00 23.33 | c . |
| MOTA | 2489 | С | PRO | C3088 | 20.931 | -14.689 | 14.822 | 1.00 20.77 | · c · |
| MOTA | 2490 | 0 | PRO | C3088 | 21.360 | -13.704 | 15.434 | 1.00 19.53 | 0 |
| ATOM | 2491 | N | TYR | C3089 | 21.647 | -15.327 | 13.903 | 1.00 18.65 | N |
| ATOM | 2492 | CA | TYR | C3089 | 22.986 | -14.869 | 13.548 | 1.00 18.94 | С |
| MOTA | 2493 | CB | TYR | C3089 | 24.015 | -15.410 | 14.557 | 1.00 19.72 | С |
| MOTA | 2494 | CG | | C3089 | | -16.891 | 14.434 | 1.00 20.97 | С |
| MOTA | 2495 | CD1 | TYR | C3089 | 25.313 | -17.360 | 13.600 | 1.00 21.58 | С |
| ATOM | 2496 | | | C3089 | | -18.721 | 13.448 | 1.00 21.20 | С |
| MOTA | 2497 | CD2 | TYR | C3089 | | -17.826 | 15.118 | 1.00 21.44 | С |
| ATOM | 2498 | CE2 | TYR | C3089 | 23.748 | -19.193 | 14.974 | 1.00 21.49 | С |
| ATOM | 2499 | CZ | TYR | C3089 | 24.764 | -19.630 | 14.133 | 1.00 20.90 | С |
| ATOM | 2500 | OH | TYR | C3089 | | -20.972 | 13.961 | 1.00 21.13 | 0 |
| MOTA | 2501 | С | TYR | C3089 | 23.310 | -15.356 | 12.142 | 1.00 19.33 | С |
| MOTA | 2502 | 0 | | C3089 | 22.695 | -16.305 | 11.658 | 1.00 18.04 | 0 |
| MOTA | 2503 | N | PHE | C3090 | 24.252 | -14.694 | 11.476 | 1.00 21.68 | N |
| MOTA | 2504 | CA | PHE | C3090 | | -15.095 | 10.129 | 1.00 22.43 | С |
| MOTA | 2505 | CB | PHE | C3090 | 25.224 | -13.921 | 9.343 | 1.00 21.81 | С |
| MOTA | 2506 | CG | | C3090 | | -13.057 | 8.686 | 1.00 22.97 | C |
| ATOM | 2507 | | | C3090 | | -11.980 | 9.364 | 1.00 22.58 | C |
| MOTA | 2508 | | | C3090 | | -13.317 | 7.382 | 1.00 22.20 | C |
| ATOM | 2509 | | | C3090 | | -11.172 | 8:752 | 1.00 21.60 | C |
| MOTA | 2510 | | | C3090 | | -12.512 | 6.762 | 1.00 21.04 | C |
| MOTA | 2511 | CZ | | C3090 | | -11.439 | 7.453 | 1.00 20.05 | C |
| ATOM | 2512 | С | | C3090 | | -16.201 | 10.185 | 1.00 23.74 | C |
| ATOM | 2513 | 0 | | C3090 | | -15.992 | 10.642 | 1.00 23.80 | 0 |
| ATOM. | 2514 | N | | C3091 | | -17.381 | 9.727 | 1.00 25.13 | N |
| MOTA | 2515 | CA | | C3091 | | -18.522 | 9.707 | 1.00 24.76 | C |
| ATOM | 2516 | СВ | | C3091 | | 3 -19.805 | 9.790 | 1.00 25.31 | C |
| ATOM | 2517 | OG | | C3091 | | -19.856 | 8.709 | 1.00 25.46 | 0 |
| MOTA | 2518 | C | | C3091 | | -18.493 | 8.393 | 1.00 25.15 | С |
| ATOM | 2519 | 0 | | C3091 | | 5 -19.075 | 8.285 | 1.00 24.95 | 0 |
| MOTA | 2520 | N | | C3092 | | 3 -17:806 | 7.401 | 1.00 25.28 | N |
| ATOM | 2521 | CA | | C3092 | | 2 -17.701 | 6.079 | 1.00 26.50 | C |
| MOTA | 2522 | CB | | C3092 | | 1 -18.759 | 5.150 | 1.00 29.33 | |
| ATOM | 2523 | CG | | C3092 | | 3 -18.723 | 3.728 | 1.00 33.15 | C |
| ATOM | 2524 | CD | | C3092 | | 3 -19.271 | 3.638 | 1.00 35.44 | 0 |
| ATOM | 2525 | | | C3092 | | 2 -18.711 | 4.204 | 1.00 36.58 1.00 37.04 | |
| ATOM | 2526 | | | C3092 | | 3 -20.384 | 2.935 | 1.00 37.04 | , N С |
| ATOM | 2527 | C | | C3092 | | 7 -16.323 | 5.465 | | |
| ATOM | 2528 | 0 | | C3092 | | 7 -15.871 | 5.365 | 1.00 24.76 1.00 24.56 | |
| MOTA | 2529 | N | ALA | C3093 | 21.86 | 4 -15.674 | 5.042 | 1.00 24.36 | į.V. |

| MOTA | 2530 | CA | ALA | C3093 | 27.801 | -14.350 | 4.422 | 1.00 24.82 | С |
|--------------|------|---------|-----|-------|--------|---------|--------|----------------|-----|
| ATOM | 2531 | CB | ALA | C3093 | 27.400 | -13.302 | 5.451 | 1.00 24.36 | C. |
| MOTA | 2532 | С | ALA | C3093 | 29.152 | -13.978 | 3.808 | 1.00 24.47 | C |
| MOTA | 2533 | 0 | ALA | C3093 | 30.200 | -14.284 | 4.365 | 1.00 24.58 | 0 |
| ATOM | 2534 | N | PRO | C3094 | 29.137 | -13.289 | 2.654 | 1.00 25.93 | N |
| ATOM | 2535 | CD | PRO | C3094 | 27.920 | -12.815 | 1.965 | 1.00 24.23 | C |
| ATOM | 2536 | CA | PRO | C3094 | 30.345 | -12.860 | 1.935 | 1.00 25.56 | C |
| ATOM | 2537 | СВ | PRO | C3094 | 29.788 | -12.404 | 0.592 | 1.00 26.20 | C |
| ATOM | 2538 | CG | | C3094 | 28.472 | -11.792 | 0.997 | 1.00 26.19 | С |
| ATOM | 2539 | С | | C3094 | 31.098 | -11.744 | 2.658 | 1.00 26.12 | С |
| ATOM | 2540 | 0 | | C3094 | | -10.703 | 2.077 | 1.00 25.63 | 0 |
| ATOM | 2541 | N | | C3095 | | -11.971 | 3.930 | 1.00 26.90 | . N |
| ATOM | 2542 | CA | | C3095 | | -10.977 | 4.739 | 1.00 26.88 | С |
| ATOM | 2543 | СВ | | C3095 | | -10.004 | 5.331 | 1.00 26.61 | С |
| ATOM | 2544 | CG | | C3095 | 31.665 | -8.923 | 6.179 | 1.00 26.50 | С |
| ATOM | 2545 | | | C3095 | 31.491 | -8.931 | 7.559 | 1.00 25.34 | С |
| ATOM | 2546 | | | C3095 | 32.406 | -7.895 | 5.601 | 1.00 26.22 | С |
| ATOM | 2547 | | | C3095 | 32.043 | | 8.350 | 1.00 24.07 | С |
| ATOM | 2548 | | | C3095 | 32.964 | | 6.384 | 1.00 25.18 | С |
| MOTA | 2549 | CZ | | C3095 | 32.781 | | 7.764 | 1.00 26.71 | С |
| ATOM | 2550 | C | | C3095 | | -11.726 | 5.841 | 1.00 27.07 | С |
| ATOM | 2551 | Ö | | C3095 | | -12.547 | 6.527 | 1.00 28.82 | 0 |
| MOTA | 2552 | N | | C3096 | | -11.450 | 6.013 | 1.00 27.08 | N |
| ATOM | 2553 | CA | | C3096 | | -12.153 | 7.022 | 1.00 26.87 | С |
| ATOM | 2554 | CB | - | C3096 | | -12.488 | 6.457 | 1.00 27.85 | C |
| ATOM | 2555 | OG | | C3096 | | -11.315 | 6.073 | 1.00 29.01 | 0 |
| ATOM | 2556 | C | | C3096 | | -11.446 | 8.364 | 1.00 27.60 | С |
| ATOM | 2557 | o | | C3096 | | -11.957 | 9.251 | 1.00 28.27 | Ō |
| ATOM | 2558 | | | C3097 | | -10.271 | 8.513 | 1.00 26.02 | N |
| | 2559 | N | | C3097 | | -9.558 | 9.775 | 1.00 25.74 | C |
| MOTA MOTA | 2560 | CA C | | C3097 | 33.406 | | 10.664 | 1.00 26.75 | Č |
| | 2561 | 0 | | C3097 | | -11.029 | 10.422 | 1.00 26.07 | 0 |
| ATOM ATOM | 2562 | Ŋ | | C3098 | 33.084 | | 11.682 | 1.00 25.99 | N |
| ATOM | 2563 | CA | | C3098 | 31.985 | | 12.572 | 1.00 26.80 | С |
| ATOM | 2564 | CB | | C3098 | 32.302 | | 13.998 | 1.00 28.83 | С |
| ATOM | 2565 | CG | | C3098 | 33.742 | | 14.383 | 1.00 33.82 | С |
| ATOM | 2566 | CD | | C3098 | 34.014 | | 15.860 | 1.00 37.34 | С |
| ATOM | 2567 | CE | | C3098 | • | -10.444 | 16.652 | 1.00 39.78 | С |
| ATOM | 2568 | NZ | | C3098 | | -10.326 | 18.084 | 1.00 40.81 | N |
| ATOM | 2569 | C | | C3098 | 30.676 | | 12.095 | 1.00 25.06 | С |
| ATOM | 2570 | Õ | | C3098 | 30.633 | | 11.670 | 1.00 24.85 | 0 |
| ATOM | 2571 | N | | C3099 | 29.611 | | 12.152 | 1.00 22.88 | N |
| ATOM | 2572 | CA | | C3099 | 28.292 | | 11.730 | 1.00 20.01 | С |
| ATOM | 2573 | CB | | C3099 | | -10.246 | 10.687 | 1.00 19.89 | С |
| ATOM | 2574 | | | C3099 | | | | 1.00 15.87 | С |
| ATOM | 2575 | | | C3099 | | -10.474 | 9.548 | 1.00 18.98 | С |
| ATOM | 2576 | | | C3099 | | -11.543 | 8.561 | 1.00 19.71 | С |
| ATOM | 2577 | C | | C3099 | 27.364 | | 12.941 | 1.00 20.05 | С |
| ATOM | 2578 | Ö | | C3099 | | -10.289 | 13.459 | 1.00 21.97 | 0 |
| ATOM | 2579 | N | | C3100 | 27.032 | | 13.398 | 1.00 18.21 | N |
| ATOM | 2580 | CA | | C3100 | 26.140 | | 14.541 | 1.00 17.20 | С |
| ATOM | 2581 | CB | | C3100 | 26.570 | | 15.383 | 1.00 17.48 | С |
| ATOM | 2582 | CG | | C3100 | 27.959 | | 15.948 | 1.00 17.00 | С |
| ATOM | 2583 | | | C3100 | 28.323 | | 17.085 | 1.00 16.80 | С |
| ATOM | 2584 | | | C3100 | 29.724 | | 17.237 | 1.00 18.05 | , c |
| ATOM | 2585 | | | C3100 | 27.599 | | 17.992 | 1.00 19.31 | C |
| ATOM | 2586 | | | C3100 | 29.119 | | 15.465 | 1.00 17.86 | С |
| 11100 | 2300 | | | 55100 | | | | - . | |

| ATOM | 2587 | NE1 | TRP | C3100 | 30.188 | -6.724 | 16.236 | 1.00 18 | .87 | | N |
|------|------|-----|-----|-------|------------------|---------|--------|---------|------|---|--------|
| ATOM | 2588 | CZ2 | TRP | C3100 | 30.417 | -8.192 | 18.263 | 1.00 19 | .19 | | С |
| MOTA | 2589 | | | C3100 | 28.290 | -9.082 | 19.012 | 1.00 19 | .20 | | С |
| MOTA | 2590 | | | C3100 | 29.687 | -8.955 | 19.136 | 1.00 17 | .94 | | С |
| MOTA | 2591 | С | | C3100 | 24.717 | -7.699 | 14.018 | 1.00 17 | | | С |
| MOTA | 2592 | | | C3100 | 24.365 | -6.656 | 13.461 | 1.00 18 | | | 0 |
| ATOM | 2593 | N | | C3101 | 23.916 | -8.742 | 14.191 | 1.00 17 | | | N |
| ATOM | 2594 | CA | | C3101 | 22.540 | -8.764 | 13.725 | 1.00 16 | | | C |
| ATOM | 2595 | CB | | C3101 | 22.321 | -9.991 | 12.837 | 1.00 16 | | | Ċ |
| ATOM | 2596 | CG | | C3101 | | -10.417 | 12.559 | 1.00 16 | | | Č |
| ATOM | 2597 | | | C3101 | 20.194 | -9.413 | 11.625 | 1.00 15 | | | Č |
| ATOM | 2598 | | | C3101 | | -11.809 | 11.939 | 1.00 18 | | | Ċ |
| ATOM | 2599 | C | | C3101 | 21.525 | -8.811 | 14.852 | 1.00 16 | | | Ċ |
| | 2600 | | | C3101 | 21.746 | -9.435 | 15.890 | 1.00 14 | | | Ö |
| MOTA | | 0 | | | 20.410 | -8.128 | 14.638 | 1.00 14 | | | N |
| ATOM | 2601 | N | | C3102 | 19.316 | -8.151 | 15.588 | 1.00 14 | | | C |
| ATOM | 2602 | CA | | | 19.424 | -7.035 | 16.619 | 1.00 14 | | | C |
| ATOM | 2603 | CB | | C3102 | | | | 1.00 14 | | | Ö |
| ATOM | 2604 | OG | | C3102 | 18.483 | -7.263 | 17.657 | | | | C |
| ATOM | 2605 | C | | C3102 | 18.052 18.020 | -7.981 | 14.761 | 1.00 14 | | | 0 |
| MOTA | 2606 | 0 | | C3102 | | -7.195 | 13.805 | 1.00 14 | | | |
| MOTA | 2607 | N | | C3103 | 17.023 | -8.734 | | | | | N C |
| MOTA | 2608 | CA | | C3103 | 15.744 | -8.710 | 14.437 | 1.00 15 | | • | C |
| ATOM | 2609 | CB | | C3103 | | -10.043 | 13.668 | 1.00 16 | | | |
| MOTA | 2610 | | | C3103 | 14.171 | -9.958 | 12.880 | 1.00 18 | | | C C |
| MOTA | 2611 | CG1 | | C3103 | | -10.353 | 12.737 | 1.00 18 | | | |
| MOTA | 2612 | | | C3103 | | -11.729 | 12.042 | 1.00 20 | | | C |
| MOTA | 2613 | С | | C3103 | 14.657 | -8.608 | 15.495 | 1.00 17 | | | C |
| ATOM | 2614 | 0 | | C3103 | 14.805 | -9.148 | 16.594 | 1.00 17 | | | 0 |
| ATOM | 2615 | N | | C3104 | 13.566 | -7.929 | 15.157 | 1.00 18 | | | N |
| MOTA | 2616 | CA | | C3104 | 12.439 | -7.798 | 16.070 | 1.00 20 | | | C |
| MOTA | 2617 | CB | | C3104 | 12.610 | -6.583 | 16.986 | 1.00 19 | | | С |
| MOTA | 2618 | OG | | C3104 | 11.596 | -6.571 | 17.981 | 1.00 23 | | | 0 |
| ATOM | 2619 | С | | C3104 | 11.188 | -7.645 | 15.214 | 1.00 22 | | | С |
| ATOM | 2620 | 0 | | C3104 | 11.269 | -7.301 | 14.033 | 1.00 22 | | | 0 |
| ATOM | 2621 | N | | C3105 | 10.028 | -7.889 | 15.796 | 1.00 23 | | | N |
| ATOM | 2622 | CA | | C3105 | 8.818 | -7.784 | 15.009 | 1.00 25 | | | C |
| ATOM | 2623 | CB | | C3105 | 8.597 | | 14.241 | 1.00 2 | | | C |
| MOTA | 2624 | CG | | C3105 | | -10.287 | 15.125 | 1.00 29 | | | C |
| MOTA | 2625 | | | C3105 | | -10.938 | 15.639 | 1.00 33 | | | С |
| ATOM | 2626 | | | C3105 | | -10.934 | 15.615 | 1.00 32 | | | N |
| MOTA | 2627 | | | C3105 | | -11.933 | 16.393 | 1.00 3 | | | С |
| MOTA | 2628 | | | C3105 | | -11.956 | 16.424 | 1.00 3 | | | N |
| MOTA | 2629 | C | | C3105 | 7.565 | | 15.805 | 1.00 2 | | | С |
| ATOM | 2630 | 0 | | C3105 | 7.499 | | 17.009 | 1.00 2 | | | 0 |
| MOTA | 2631 | N | | C3106 | 6.575 | | 15.086 | 1.00 2 | | | N |
| MOTA | 2632 | CA | | C3106 | 5.261 | -6.652 | 15.613 | 1.00 3 | | | C |
| MOTA | 2633 | CB | | C3106 | 4.855 | | 15.300 | 1.00 3 | | | C |
| ATOM | 2634 | OG1 | THR | C3106 | 4.804 | -5:030 | 13.878 | 1.00 3 | | | 0 |
| ATOM | 2635 | CG2 | | C3106 | 5.848 | | 15.905 | 1.00 3 | | | С |
| ATOM | 2636 | С | | C3106 | 4.332 | | 14.840 | 1.00 3 | | | C |
| MOTA | 2637 | 0 | | C3106 | 4.792 | | 14.101 | 1.00 3 | | | 0 |
| MOTA | 2638 | N | | C3107 | 3.031 | | 14.987 | 1.00 3 | | | N |
| MOTA | 2639 | CA | | C3107 | 2.056 | | 14.296 | 1.00 3 | | | С |
| ATOM | 2640 | CB | ASP | C3107 | 0.674 | | 14.934 | 1.00 3 | | | С |
| ATOM | 2641 | CG | ASP | C3107 | 0.596 | | 16.327 | 1.00 4 | | | С |
| MOTA | 2642 | OD1 | ASP | C3107 | -0.205 | -8.097 | 17.136 | 1.00 4 | | | 0 |
| MOTA | 2643 | OD2 | ASP | C3107 | 1.319 | -9.591 | 16.612 | 1.00 4 | 4.36 | | 0 |
| | | | | | | | | | | | |

| ATOM | 2644 | С | ASP | C3107 | 1.959 | -7.890 | 12.807 | 1.00 31.24 | С |
|--------------|--------------|--------|-----|----------------|------------------|---------------------|------------------|--------------------------|--------|
| ATOM | 2645 | 0 | ASP | C3107 | 1.521 | -8.729 | 12.026 | 1.00 32.84 | 0 |
| ATOM | 2646 | N | GLN | C3108 | 2.374 | -6.690 | 12.410 | 1.00 28.20 | N |
| MOTA | 2647 | | | C3108 | 2.284 | -6.289 | 11.009 | 1.00 27.03 | C |
| ATOM | 2648 | | | C3108 | 1.590 | -4.928 | 10.877 | 0.05 26.57 | · c |
| ATOM | 2649 | CG | | C3108 | 0.284 | -4.788 | 11.626 | 0.05 26.25 | С |
| MOTA | 2650 | CD | | C3108 | 0.486 | -4.733 | 13.121 | 0.05 26.05 | С |
| MOTA | 2651 | | | C3108 | 1.220 | -3.887 | 13.631 | 0.05 25.96 | 0 |
| MOTA | 2652 | | | C3108 | -0.165 | -5.636 | 13.834 | 0.05 25.84 | N |
| ATOM | 2653 | C | | C3108 | 3.607 | -6.204 | 10.264 | 1.00 25.37 | C |
| ATOM | 2654 | 0 | | C3108 | 3.624 | -6.210 | 9.032 | 1.00 24.85 | 0 |
| ATOM | 2655 | N | | C3109 | 4.716 | -6.098 | 10.987 | 1.00 24.20 | N C |
| ATOM | 2656 | CA | | C3109 | 5.996 | -5.994 | 10.299 | 1.00 23.19 1.00 24.65 | С |
| ATOM | 2657 | CB | | C3109 | 6.210 | -4.548 | 9.827 | 1.00 24.03 | C |
| ATOM | 2658 | CG | | C3109 | 6.268 7.406 | -3.541 -3.421 | 10.947 11.738 | 1.00 26.19 | C |
| MOTA | 2659 | | | C3109 | 5.181 | -2.714 | 11.738 | 1.00 27.63 | č |
| MOTA | 2660 2661 | | | C3109 | 7.464 | -2.490 | 12.780 | 1.00 26.39 | č |
| ATOM | 2662 | | | C3109 | 5.225 | -1.780 | 12.249 | 1.00 28.63 | Ċ |
| ATOM ATOM | 2663 | CZ | | C3109 | 6.371 | -1.669 | 13.036 | 1.00 28.60 | Č |
| ATOM | 2664 | C | | C3109 | 7.191 | -6.459 | 11.116 | 1.00 21.14 | c |
| ATOM | 2665 | 0 | | C3109 | 7.100 | -6.648 | 12.328 | 1.00 19.22 | 0 |
| ATOM | 2666 | N | | C3110 | 8.308 | -6.650 | 10.425 | 1.00 19.26 | N |
| ATOM | 2667 | CA | | C3110 | 9.550 | -7.083 | 11.052 | 1.00 19.85 | С |
| ATOM | 2668 | CB | | C3110 | 10.027 | -8.438 | 10.471 | 1.00 21.25 | С |
| ATOM | 2669 | | | C3110 | 11.360 | -8.859 | 11.101 | 1.00 23.25 | С |
| ATOM | 2670 | | | C3110 | 8.980 | -9.488 | 10.719 | 1.00 25.17 | С |
| ATOM | 2671 | C | | C3110 | 10.604 | -6.039 | 10.737 | 1.00 19.21 | C |
| ATOM | 2672 | 0 | VAL | C3110 | 10.503 | -5.345 | 9.725 | 1.00 19.53 | 0 |
| MOTA | 2673 | N | THR | C3111 | 11.603 | -5. 9 25 | 11.608 | 1.00 19.09 | N |
| MOTA | 2674 | CA | THR | C3111 | 12.695 | -4.984 | 11.409 | 1.00 20.72 | С |
| MOTA | 2675 | CB | THR | C3111 | 12.608 | -3.765 | 12.368 | 1.00 22.75 | С |
| MOTA | 2676 | OG1 | THR | C3111 | 12.635 | -4.216 | 13.730 | 1.00 26.03 | 0 |
| MOTA | 2677 | CG2 | | C3111 | 11.322 | -2.976 | 12.124 | 1.00 22.96 | C |
| ATOM | 2678 | С | | C3111 | 13.993 | -5.725 | 11.684 | 1.00 20.16 | С |
| ATOM | 2679 | 0 | | C3111 | 14.024 | -6.664 | 12.481 | 1.00 20.27 | 0 |
| MOTA | 2680 | N | | C3112 | 15.060 | -5.312 | 11.010 | 1.00 19.72 | N C |
| MOTA | 2681 | CA | | C3112 | 16.361 | -5.935 | 11.201 | 1.00 19.77 | C |
| ATOM | 2682 | CB | | C3112 | 16.617 | -6.975 -4.868 | 10.109 | 1.00 18.61 1.00 19.41 | C |
| ATOM | 2683 | C | | C3112 | 17.441 17.337 | -3.885 | 11.172 10.442 | 1.00 19.41 | Ö |
| ATOM | 2684 2685 | O N | | C3112 C3113 | 18.474 | -5.062 | 11.980 | 1.00 20.21 | N |
| ATOM ATOM | 2686 | CA | | C3113 | 19.579 | -4.124 | 12.045 | 1.00 18.53 | C |
| ATOM | 2687 | CB | | C3113 | 19.506 | -3.298 | 13.327 | 1.00 19.50 | С |
| MOTA | 2688 | OG | | C3113 | | -2.293 | | | 0 |
| ATOM | 2689 | C | | C3113 | 20.888 | -4.895 | 12.003 | 1.00 18.71 | C |
| ATOM | 2690 | 0 | | C3113 | 21.084 | -5.843 | 12.767 | 1.00 16.55 | 0 |
| ATOM | 2691 | N | | C3114 | 21.779 | -4:472 | 11.107 | 1.00 17.09 | N |
| ATOM | 2692 | CA | | C3114 | 23.071 | -5.115 | 10.930 | 1.00 17.37 | C |
| MOTA | 2693 | CB | VAL | C3114 | 23.145 | -5.842 | 9.563 | 1.00 16.61 | С |
| ATOM | 2694 | CG1 | VAL | C3114 | 24.593 | -6.263 | 9.255 | 1.00 18.34 | С |
| ATOM' | 2695 | CG2 | | C3114 | 22.244 | - 7.050 | 9.576 | 1.00 16.94 | C |
| MOTA | 2696 | С | VAL | C3114 | 24.216 | -4.116 | 10.993 | 1.00 16.94 | C |
| MOTA | 2697 | 0 | | C3114 | 24.145 | -3.043 | 10.408 | 1.00 16.28 | 0 |
| MOTA | 2698 | N | | C3115 | 25.265 | -4.477 | 11.720 | 1.00 17.86 | N |
| ATOM | 2699 | CA | | C3115 | 26.446 | -3.632 | 11.820 | 1.00 19.21 | C |
| ATOM | 2700 | CB | ILE | C3115 | 26.667 | -3.085 | 13,253 | 1.00 19.71 | С |

| ATOM | 2701 | CG2 | ILE | C3115 | 27.926 | -2.217 | 13.287 | 1.00 1 | | C |
|------|------|-----|------|-------|--------|---------|--------|--------|-------|---|
| ATOM | 2702 | CG1 | ILE | C3115 | 25.451 | -2.268 | 13.703 | 1.00 1 | 9.12 | С |
| ATOM | 2703 | CD1 | ILE | C3115 | 25.573 | -1.701 | 15.110 | 1.00 2 | 0.38 | С |
| ATOM | 2704 | С | ILE | C3115 | 27.627 | -4.516 | 11.440 | 1.00 1 | | С |
| MOTA | 2705 | 0 | ILE | C3115 | 27.806 | -5.589 | 12.007 | 1.00 1 | 8.31 | 0 |
| MOTA | 2706 | N | LEU | C3116 | 28.409 | -4.076 | 10.457 | 1.00 1 | 9.22 | N |
| ATOM | 2707 | CA | LEU | C3116 | 29.578 | -4.830 | 10.021 | 1.00 2 | 0.77 | С |
| ATOM | 2708 | CB | | C3116 | 29.696 | -4.805 | 8.493 | 1.00 2 | 0.70 | С |
| ATOM | 2709 | CG | | C3116 | 28.445 | -5.235 | 7.703 | 1.00 1 | 9.25 | С |
| ATOM | 2710 | | | C3116 | 28.758 | -5.249 | 6.218 | 1.00 2 | 1.02 | С |
| ATOM | 2711 | | | C3116 | 27.996 | -6.614 | 8.150 | 1.00 1 | | С |
| ATOM | 2712 | C | | C3116 | 30.803 | -4.182 | 10.655 | 1.00 2 | 1.44 | С |
| ATOM | 2713 | ō | | C3116 | 30.996 | -2.969 | 10.554 | 1.00 2 | | 0 |
| ATOM | 2714 | N | | C3117 | 31.620 | -4.994 | 11.314 | 1.00 2 | | N |
| ATOM | 2715 | CA | | C3117 | 32.812 | -4.493 | 11.987 | 1.00 2 | | С |
| ATOM | 2716 | CB | | C3117 | 32.571 | -4.457 | 13.504 | 1.00 2 | 7.48 | С |
| ATOM | 2717 | CG | | C3117 | 33.817 | -4.166 | 14.343 | 1.00 3 | | С |
| ATOM | 2718 | CD | | C3117 | 33.628 | -4.470 | 15.826 | 1.00 2 | | С |
| MOTA | 2719 | | | C3117 | 33.182 | -5.595 | 16.158 | 1.00 2 | | 0 |
| ATOM | 2720 | | | C3117 | 33.932 | -3.585 | 16.660 | 1.00 2 | | 0 |
| ATOM | 2721 | C | | C3117 | 34.048 | -5.335 | 11.680 | 1.00 2 | | С |
| ATOM | 2722 | Ö | | C3117 | 33.978 | -6.563 | 11.578 | 1.00 2 | | 0 |
| ATOM | 2723 | N | | C3118 | 35.178 | -4.657 | 11.513 | 1.00 3 | | N |
| ATOM | 2724 | CA | | C3118 | 36.446 | -5.323 | 11.248 | 1.00 3 | | С |
| ATOM | 2725 | CB | | C3118 | 37.015 | -4.880 | 9.893 | 1.00 3 | | C |
| ATOM | 2726 | CG | | C3118 | 36.592 | -5.772 | 8.727 | 1.00 4 | | С |
| MOTA | 2727 | CD | | C3118 | 37.041 | -5.248 | 7.368 | 1.00 4 | | С |
| ATOM | 2728 | | | C3118 | 38.193 | -4.776 | 7.253 | 1.00 4 | | ō |
| ATOM | 2729 | | | C3118 | 36.242 | -5.321 | 6.409 | 1.00 4 | | Ō |
| ATOM | 2730 | C | | C3118 | 37.414 | -4.963 | 12.369 | 1.00 | | Ċ |
| ATOM | 2731 | 0 | | C3118 | 37.417 | -3.784 | 12.785 | 1.00 3 | | Ó |
| ATOM | 2732 | | | C3118 | 38.154 | -5.858 | 12.821 | 1.00 3 | | Ō |
| TER | 2732 | OAI | | C3118 | 30.134 | 3.030 | 12.021 | 1.00 | 30.00 | • |
| ATOM | 2734 | 0 | | W4002 | 24.915 | 17.154 | 36.149 | 1.00 2 | 24.34 | 0 |
| ATOM | 2735 | Ö | | W4002 | 1.430 | 5.412 | 7.521 | 1.00 2 | | Ō |
| MOTA | 2736 | 0 | | W4003 | | -11.883 | 17.512 | 1.00 2 | | Ō |
| ATOM | 2737 | Ö | | W4006 | 20.551 | 4.946 | 39.709 | 1.00 | | Ō |
| ATOM | 2738 | o | | W4008 | 0.497 | 12.883 | 37.515 | 1.00 | | 0 |
| ATOM | 2739 | Ö | | W4009 | 22.219 | 1.070 | 4.722 | 1.00 | | Ó |
| MOTA | 2740 | Ö | | W4010 | 23.057 | | 27.783 | 1.00 | | 0 |
| ATOM | 2741 | o | | W4012 | 26.158 | 9.664 | 6.047 | 1.00 | | 0 |
| ATOM | 2742 | Ö | | W4013 | | -14.652 | 11.137 | 1.00 | | 0 |
| ATOM | 2743 | Ö | | W4014 | | -19.177 | 9.562 | 1.00 | | 0 |
| ATOM | 2744 | ŏ | | W4016 | 11.365 | 8.055 | -2.295 | 1.00 | 29.34 | 0 |
| ATOM | 2745 | | | W4017 | | 7.951 | | | | 0 |
| ATOM | 2746 | ŏ | | W4018 | 20.734 | 17.150 | 36.413 | 1.00 | | 0 |
| ATOM | 2747 | Ö | | W4020 | -9.281 | -6.387 | 41.928 | 1.00 | | 0 |
| ATOM | 2748 | o | | W4021 | | -12:662 | 22.632 | 1.00 | | 0 |
| ATOM | 2749 | Ö | | W4025 | 18.802 | 13.286 | -2.320 | 1.00 | | 0 |
| ATOM | 2750 | Ö | | W4026 | 26.500 | 16.583 | 31.811 | 1.00 | | 0 |
| ATOM | 2751 | Ö | | W4027 | 6.858 | -4.124 | 3.265 | 1.00 | | 0 |
| ATOM | 2752 | Ö | | W4028 | 10.702 | 1.088 | -3.405 | 1.00 | | 0 |
| MOTA | 2753 | 0 | _ | W4029 | 12.811 | | 27.541 | 1.00 | | Ō |
| MOTA | 2754 | 0 | | W4031 | 12.749 | | 19.973 | 1.00 | | 0 |
| ATOM | 2755 | 0 | | W4031 | 13.535 | | 2.032 | | 40.39 | Ö |
| ATOM | 2756 | Ö | | W4033 | 13.594 | | 33.675 | | 30.23 | 0 |
| ATOM | 2757 | Ö | | W4035 | 10.527 | | 27.661 | | 22.20 | Ö |
| VION | 2131 | 9 | 1101 | | 10.327 | 3.020 | 2001 | | | - |

| MOTA | 2758 | 0 | HOH W4038 | 10.071 6.775 24.507 1.00 34.64 | 0 |
|------|------|---|-----------|----------------------------------|-----|
| MOTA | 2759 | 0 | HOH W4039 | 22.581 2.348 2.717 1.00 30.28 | 0 |
| MOTA | 2760 | 0 | HOH W4041 | 34.765 -18.840 6.665 1.00 52.31 | 0 |
| MOTA | 2761 | 0 | HOH W4042 | 19.832 10.430 22.362 1.00 30.27 | 0 |
| ATOM | 2762 | 0 | HOH W4043 | 25.556 -0.749 36.545 1.00 47.38 | 0 |
| MOTA | 2763 | 0 | HOH W4044 | 1.280 -1.711 37.119 1.00 35.25 | 0 |
| ATOM | 2764 | 0 | HOH W4045 | 23.055 -3.951 37.102 1.00 29.32 | 0 |
| MOTA | 2765 | 0 | HOH W4046 | 10.346 9.220 18.446 1.00 31.53 | 0 |
| ATOM | 2766 | 0 | HOH W4047 | -3.287 0.403 31.271 1.00 53.94 | 0 |
| ATOM | 2767 | 0 | HOH W4048 | 4.921 -2.235 2.298 1.00 35.71 | 0 |
| ATOM | 2768 | 0 | HOH W4050 | 4.512 -5.663 22.584 1.00 34.27 | 0 |
| ATOM | 2769 | 0 | HOH W4051 | 32.165 -16.448 3.541 1.00 29.46 | 0 |
| MOTA | 2770 | 0 | HOH W4052 | 17.356 -10.554 17.298 1.00 20.37 | 0 |
| ATOM | 2771 | 0 | HOH W4053 | 23.079 8.307 36.567 1.00 27.23 | 0 |
| ATOM | 2772 | 0 | HOH W4054 | 22.333 9.961 24.703 1.00 41.93 | 0 |
| ATOM | 2773 | 0 | HOH W4055 | 19.848 3.106 3.638 1.00 23.68 | 0 |
| ATOM | 2774 | 0 | HOH W4056 | 14.228 9.547 2.164 1.00 13.78 | 0 |
| ATOM | 2775 | 0 | HOH W4057 | -5.992 9.409 37.088 1.00 40.47 | 0 |
| MOTA | 2776 | 0 | HOH W4058 | 15.141 2.885 1.432 1.00 32.54 | 0 |
| MOTA | 2777 | 0 | HOH W4059 | 27.207 3.715 -0.205 1.00 38.02 | 0 |
| ATOM | 2778 | 0 | HOH W4060 | 4.520 8.617 13.683 1.00 29.66 | 0 |
| ATOM | 2779 | 0 | HOH W4061 | -0.534 22.844 0.843 1.00 43.95 | 0 |
| MOTA | 2780 | 0 | HOH W4062 | 33.271 0.399 4.561 1.00 41.51 | 0 |
| MOTA | 2781 | 0 | HOH W4063 | 10.750 -9.990 18.523 1.00 37.79 | 0 |
| MOTA | 2782 | 0 | HOH W4065 | 35.003 2.841 10.072 1.00 34.95 | 0 |
| ATOM | 2783 | 0 | HOH W4066 | 15.619 13.987 20.059 1.00 51.87 | 0 |
| ATOM | 2784 | 0 | HOH W4067 | 30.322 -16.861 5.985 1.00 25.67 | 0 |
| ATOM | 2785 | 0 | HOH W4068 | -3.928 16.855 6.776 1.00 37.28 | 0 |
| ATOM | 2786 | 0 | HOH W4069 | 20.489 9.067 39.451 1.00 48.83 | 0 |
| MOTA | 2787 | 0 | HOH W4070 | 38.865 -2.991 24.079 1.00 52.94 | 0 |
| MOTA | 2788 | 0 | HOH W4071 | 18.289 12.534 22.275 1.00 32.83 | 0 |
| ATOM | 2789 | 0 | HOH W4072 | 16.738 0.024 14.519 1.00 34.01 | 0 |
| ATOM | 2790 | 0 | HOH W4073 | 1.959 -19.500 14.371 1.00 40.61 | 0 |
| MOTA | 2791 | 0 | HOH W4074 | 1.805 -19.989 7.096 1.00 40.73 | 0 |
| MOTA | 2792 | 0 | HOH W4075 | 15.612 10.434 34.742 1.00 32.10 | 0 |
| MOTA | 2793 | 0 | HOH W4076 | 13.088 0.232 13.391 1.00 37.71 | 0 |
| ATOM | 2794 | 0 | HOH W4077 | -3.125 13.706 3.280 1.00 34.62 | 0 |
| ATOM | 2795 | 0 | HOH W4078 | 2.257 8.002 15.256 1.00 30.49 | 0 |
| MOTA | 2796 | 0 | HOH W4079 | 1.805 3.820 14.707 1.00 34.86 | 0 |
| MOTA | 2797 | 0 | HOH W4080 | 5.391 -8.908 -2.363 1.00 35.80 | 0 |
| MOTA | 2798 | 0 | HOH W4081 | 13.173 18.130 19.444 1.00 42.58 | 0 |
| MOTA | 2799 | 0 | HOH W4083 | 3.428 25.760 7.166 1.00 47.46 | 0 |
| MOTA | 2800 | 0 | HOH W4085 | 19.600 0.144 14.509 1.00 27.27 | 0 |
| ATOM | 2801 | 0 | HOH W4086 | 17.905 -21.379 25.352 1.00 38.73 | 0 |
| ATOM | 2802 | 0 | HOH W4087 | 33.360 5.719 22.662 1.00 36.03 | 0 |
| MOTA | 2803 | 0 | HOH W4089 | 9.617 -0.859 41.147 1.00 32.45 | 0 |
| MOTA | 2804 | 0 | HOH W4090 | 28.109 -16.115 0.982 1.00 29.92 | 0 |
| ATOM | 2805 | 0 | HOH W4091 | 38.387 -10.896 9.764 1.00 47.94 | 0 |
| MOTA | 2806 | 0 | HOH W4092 | 5.988 24.794 8.424 1.00 43.14 | 0 |
| MOTA | 2807 | 0 | | -3.277 6.265 6.376 1.00 35.40 | 0 |
| ATOM | 2808 | 0 | HOH W4094 | 30.455 10.041 6.941 1.00 32.99 | 0 |
| ATOM | 2809 | 0 | HOH W4095 | 26.815 0.664 4.954 1.00 27.85 | 0 |
| MOTA | 2810 | О | HOH W4096 | 15.273 23.735 -4.277 1.00 47.73 | 0 |
| MOTA | 2811 | 0 | HOH W4099 | 26.449 1.509 2.656 1.00 65.15 | 0 |
| MOTA | 2812 | | HOH W4100 | 0.838 7.963 3.230 1.00 37.27 | 0 |
| ATOM | 2813 | | HOH W4101 | 29.381 8.723 0.899 1.00 43.02 | . 0 |
| ATOM | 2814 | 0 | HOH W4102 | 40.660 -5.785 23.570 1.00 45.63 | Ü |
| | | | | | |

| ATOM | 2815 | 0 | HOH W4103 | 26.328 6.312 5.240 1.00 53.4 | |
|--------------|--------------|---|------------------------|---|-------------|
| ATOM | 2816 | 0 | HOH W4104 | 34.720 1.902 16.155 1.00 43.8 | |
| ATOM | 2817 | 0 | HOH W4105 | -7.319 -8.388 40.539 1.00 39.0 | |
| ATOM | 2818 | 0 | HOH W4106 | 18.869 25.116 1.680 1.00 46.3 | |
| ATOM | 2819 | 0 | HOH W4107 | 16.340 14.706 24.191 1.00 38.0 | |
| MOTA | 2820 | 0 | HOH W4108 | 6.923 8.908 27.885 1.00 36.2 | |
| ATOM | 2821 | 0 | HOH W4109 | 12.525 -11.624 17.355 1.00 34.5 | |
| MOTA | 2822 | 0 | HOH W4110 | 34.314 -7.049 18.369 1.00 34.6 | |
| ATOM | 2823 | 0 | HOH W4113 | 38.750 -2.512 27.167 1.00 57.8 | |
| ATOM | 2824 | 0 | HOH W4114 | 18.115 3.750 1.319 1.00 31.4 | |
| MOTA | 2825 | 0 | HOH W4115 | 27.875 1.248 31.553 1.00 55.1 | |
| MOTA | 2826 | 0 | HOH W4116 | 7.683 -21.130 -8.639 1.00 46.3 | |
| ATOM | 2827 | 0 | HOH W4117 | -0.188 6.861 39.329 1.00 45.2 | |
| MOTA | 2828 | 0 | HOH W4118 | 15.597 2.256 13.150 1.00 38.6 | |
| ATOM | 2829 | 0 | HOH W4120 | 29.648 18.094 28.167 1.00 35.9 | |
| ATOM | 2830 | 0 | HOH W4121 | 16.930 -20.733 11.766 1.00 37.4 | |
| ATOM | 2831 | 0 | HOH W4122 | 7.167 -12.636 -7.617 1.00 48.6 | |
| ATOM | 2832 | 0 | HOH W4123 | 37.628 10.036 12.640 1.00 43. | |
| MOTA | 2833 | 0 | HOH W4124 | 13.082 -13.269 27.306 1.00 52.3 | |
| ATOM | 2834 | 0 | HOH W4125 | 4.976 -26.696 6.493 1.00 47.3 | |
| MOTA | 2835 | 0 | HOH W4126 | 2.241 -22.225 15.163 1.00 51. | |
| MOTA | 2836 | 0 | HOH W4127 | 8.988 -10.057 20.455 1.00 50. | |
| ATOM | 2837 | 0 | HOH W4128 | 18.719 -13.639 -6.616 1.00 49. | |
| ATOM · | 2838 | 0 | HOH W4129 | 21.651 22.882 0.638 1.00 46. | |
| MOTA | 2839 | 0 | HOH W4130 | 27.239 3.345 29.234 1.00 25. | |
| MOTA | 2840 | 0 | HOH W4131 | 9.016 -8.748 -1.209 1.00 45. | |
| ATOM | 2841 | 0 | HOH W4132 | 13.082 -9.632 37.155 1.00 43. | |
| MOTA | 2842 | 0 | HOH W4133 | 29.378 15.689 6.467 1.00 49. | |
| MOTA | 2843 | 0 | HOH W4134 | -7.908 -3.988 42.818 1.00 30. | |
| MOTA | 2844 | 0 | HOH W4135 | 3.562 -8.297 27.665 1.00 45. | |
| ATOM | 2845 | 0 | HOH W4136 | -7.199 -0.161 28.514 1.00 24. | |
| ATOM | 2846 | 0 | HOH W4137 | 31.194 6.207 6.288 1.00 42. | |
| ATOM | 2847 | 0 | HOH W4138 | 19.383 8.002 23.933 1.00 35. | |
| MOTA | 2848 | 0 | HOH W4139 | -6.335 -8.439 24.417 1.00 47. | |
| ATOM | 2849 | 0 | HOH W4140 | 37.800 -1.901 17.636 1.00 38. | |
| ATOM | 2850 | 0 | HOH W4141 | 36.896 4.279 13.213 1.00 44. 18.980 16.923 -5.091 1.00 32. | |
| MOTA | 2851 | 0 | HOH W4142 | | |
| MOTA | 2852 | 0 | HOH W4143 | 6.338 17.886 -7.468 1.00 44. 8.099 9.789 -8.452 1.00 34. | |
| ATOM | 2853 | 0 | HOH W4144 | | |
| ATOM | 2854 | 0 | HOH W4145 | | |
| ATOM | 2855 | 0 | HOH W4146 | | |
| MOTA | 2856 | 0 | HOH W4147 | 28.353 11.186 5.638 1.00 36. 0.018 1.428 9.817 1.00 46. | |
| ATOM | 2857 | 0 | HOH W4148 | 38.727 -0.038 26.083 1.00 50. | |
| ATOM | 2858 | 0 | HOH W4149 | 24.171 -8.880 20.179 1.00 43. | _ |
| ATOM | 2859 | 0 | HOH W4150 HOH W4151 | -0.768 -7.980 41.105 1.00.48. | _ |
| ATOM | 2860 | 0 | | 26.257 -5.046 35.426 1.00 48. | |
| ATOM | 2861 2862 | 0 | HOH W4152 HOH W4153 | 35.432 0.075 28.104 1.00 43. | |
| MOTA MOTA | 2863 | 0 | HOH W4154 | 35.301 2.870 27.050 1.00 52. | |
| | | | HOH W4154 | -4.097 3.796 17.913 1.00 44 | |
| ATOM ATOM | 2864 2865 | 0 | HOH W4156 | 29.195 0.822 3.786 1.00 40 | |
| ATOM | 2866 | 0 | HOH W4157 | 15.774 -2.195 11.976 1.00 39 | |
| ATOM | 2867 | Ö | HOH W4158 | 22.736 4.680 3.551 1.00 24 | |
| ATOM | 2868 | 0 | HOH W4159 | 10.086 -24.038 17.929 1.00 54 | |
| ATOM | 2869 | | HOH W4161 | 37.774 -8.164 11.579 1.00 59 | |
| ATOM | 2870 | | HOH W4162 | 25.882 18.452 33.331 1.00.33 | |
| ATOM | 2871 | | HOH W4163 | -0.430 0.356 12.041 1.00 45 | |
| ALON | 2011 | ~ | ,,,,,,,, | | |

| ATOM | 2872 | 0 | HOH W4164 | -3.073 | -7.128 | 24.073 | 1.00 45.12 | 0 |
|------|------|---|-----------|--------|---------|--------|------------|---|
| ATOM | 2873 | 0 | HOH W4165 | 31.655 | 13.815 | 8.848 | 1.00 29.05 | 0 |
| ATOM | 2874 | Ó | HOH W4166 | 17.133 | 8.014 | -0.782 | 1.00 24.81 | 0 |
| ATOM | 2875 | Ō | HOH W4167 | 11.582 | -12.517 | 13.880 | 1.00 37.19 | 0 |
| ATOM | 2876 | 0 | HOH W4168 | 15.057 | -15.827 | 14.902 | 1.00 25.73 | 0 |
| ATOM | 2877 | 0 | HOH W4169 | 12.130 | -17.876 | 15.236 | 1.00 35.36 | 0 |
| ATOM | 2878 | 0 | HOH W4170 | 7.663 | 8.075 | 46.234 | 1.00 31.45 | 0 |
| ATOM | 2879 | 0 | HOH W4171 | 8.858 | 17.412 | 12.301 | 1.00 37.47 | 0 |
| TER | 2880 | · | HOH W4171 | | | | | |
| END | | | | | | | | |
| | | | | | | | | |

TABLE 5

```
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.90 A
REMARK starting r= 0.2427 free_r= 0.2720
REMARK final r= 0.2425 free r= 0.2731
REMARK B rmsd for bonded mainchain atoms= 0.960 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 1.085 target= 2.0 REMARK B rmsd for angle mainchain atoms= 1.688 target= 2.0
REMARK B rmsd for angle sidechain atoms= 1.768 target= 2.5
REMARK wa= 1.18715
REMARK rweight=0.298329
REMARK target= mlf steps= 30
REMARK sg= C2 a= 120.188 b= 62.273 c= 51.673 alpha= 90 beta= 98.745 gamma= 90
REMARK parameter file 1 : CNX_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNX_TOPPAR:water_rep.param
REMARK parameter file 3 : CNX_TOPPAR:ion.param
REMARK parameter file 4 : 35-ADP/35-ADP.param
REMARK molecular structure file: generate.psf
REMARK input coordinates: minimize.pdb
REMARK reflection file= ../data/x-ray_data.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.90
REMARK initial B-factor correction applied to fobs :
REMARK B11= 0.036 B22= -2.635 B33= 2.599
REMARK B12= 0.000 B13= 0.515 B23= 0.000
REMARK B-factor correction applied to coordinate array B: 0.030
REMARK bulk solvent: (Mask) density level= 0.369861 e/A^3, B-factor= 96.7512 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range:
                                                                                                   29870 ( 100.0 % )
                                                                                                   330 ( 1.1 % )
REMARK number of unobserved reflections (no entry or |F|=0):
                                                                                                                 0.0 % }
 REMARK number of reflections rejected:
                                                                                                       0 (
                                                                                                   29540 ( 98.9 % )
REMARK total number of reflections used:
                                                                                                   28083 ( 94.0 % )
 REMARK number of reflections in working set:
                                                                                                   1457 ( 4.9 %)
 REMARK number of reflections in test set:
 REMARK FILENAME="acps 35-ADP.pdb"
 REMARK Written by CNX VERSION:2000
          1 CB MET A1003 37.264 5.634 20.230 1.00 26.46
2 CG MET A1003 36.648 6.209 21.498 1.00 29.51
 MOTA
 MOTA
                                                   37.784 7.312 22.398 1.00 33.70
37.843 8.718 21.291 1.00 32.08
               3 SD MET A1003
 ATOM
ATOM 4 CE MET A1003 37.843 8.718 21.291 1.00 32.08
ATOM 5 C MET A1003 35.048 5.262 19.102 1.00 23.04
ATOM 6 O MET A1003 35.009 6.245 18.358 1.00 22.46
ATOM 7 N MET A1003 37.108 4.155 18.256 1.00 24.80
ATOM 8 CA MET A1003 36.389 4.622 19.479 1.00 24.32
ATOM 9 N ILE A1004 33.957 4.690 19.606 1.00 22.15
ATOM 10 CA ILE A1004 32.606 5.202 19.348 1.00 21.16
ATOM 11 CB ILE A1004 31.535 4.120 19.670 1.00 21.51
ATOM 12 CG2 ILE A1004 30.122 4.710 19.558 1.00 21.66
ATOM 13 CG1 ILE A1004 31.696 2.927 18.722 1.00 21.75
ATOM 14 CD1 ILE A1004 30.823 1.734 19.074 1.00 22.20
ATOM 15 C ILE A1004 32.361 6.417 20.245 1.00 20.57
ATOM 16 O ILE A1004 32.773 6.416 21.407 1.00 21.36
ATOM 17 N VAL A1005 31.705 7.448 19.713 1.00 19.47
ATOM 18 CA VAL A1005 31.409 8.652 20.492 1.00 18.73
ATOM 19 CB VAL A1005 32.308 9.852 20.042 1.00 19.66
ATOM 20 CG1 VAL A1005 33.779 9.530 20.319 1.00 20.39
 ATOM
              4 CE MET A1003
                                                                                                                           0
                                                                                                                           N
                                                                                                                           N
                                                                                                                           С
                                                                                                                           С
                                                                                                                          С
```

| | | | | | | | | 4 00 00 00 | |
|---------|----|-----|-------|-------|--------|--------|--------|------------|-----|
| ATOM | 21 | CG2 | VAL . | A1005 | 32.119 | 10.142 | 18.562 | 1.00 20.39 | C |
| ATOM | 22 | С | VAL . | A1005 | 29.924 | 9.085 | 20.502 | 1.00 17.55 | С |
| ATOM | 23 | 0 | VAL . | A1005 | 29.601 | 10.193 | 20.940 | 1.00 16.98 | 0 |
| ATOM | 24 | N | GLY . | A1006 | 29.026 | 8.207 | 20.041 | 1.00 16.14 | N |
| ATOM | 25 | CA | GLY | A1006 | 27.593 | 8.513 | 20.046 | 1.00 14.83 | C |
| ATOM | 26 | | | A1006 | 26.725 | 7.566 | 19.216 | 1.00 13.78 | С |
| ATOM | 27 | | | A1006 | 27.223 | 6.982 | 18.257 | 1.00 12.47 | 0 |
| ATOM | 28 | N | | A1007 | 25.442 | 7.409 | 19.581 | 1.00 13.88 | N |
| ATOM | 29 | CA | | A1007 | 24.495 | 6.535 | 18.844 | 1.00 14.19 | С |
| | | | | A1007 | 24.638 | 5.080 | 19.332 | 1.00 14.36 | С |
| ATOM | 30 | CB | | | 23.663 | 4.115 | 18.711 | 1.00 14.94 | Ċ |
| ATOM | 31 | CG | | A1007 | 22.904 | 3.137 | 19.266 | 1.00 15.52 | c |
| ATOM | 32 | | | A1007 | | 4.070 | 17.355 | 1.00 13.32 | N |
| ATOM | 33 | | | A1007 | 23.410 | | | 1.00 14.28 | Č |
| ATOM | 34 | | | A1007 | 22.537 | 3.108 | 17.102 | | N |
| ATOM | 35 | | | A1007 | 22.214 | 2.526 | 18.245 | 1.00 15.49 | |
| MOTA | 36 | С | | A1007 | 23.025 | 7.000 | 18.999 | 1.00 13.90 | С |
| MOTA | 37 | 0 | | A1007 | 22.588 | 7.310 | 20.115 | 1.00 13.25 | 0 |
| MOTA | 38 | N | | A1008 | 22.276 | 7.053 | 17.888 | 1.00 13.72 | N |
| ATOM | 39 | CA | GLY | A1008 | 20.870 | 7.476 | 17.931 | 1.00 13.61 | C |
| ATOM | 40 | С | | A1008 | 19.944 | 6.833 | 16.890 | 1.00 13.86 | C |
| ATOM | 41 | 0 | GLY | A1008 | 20.402 | 6.498 | 15.795 | 1.00 13.86 | 0 |
| ATOM | 42 | N | ILE | A1009 | 18.653 | 6.649 | 17.218 | 1.00 13.29 | N |
| ATOM | 43 | CA | ILE | A1009 | 17.672 | 6.046 | 16.281 | 1.00 13.44 | С |
| ATOM | 44 | CB | ILE | A1009 | 17.342 | 4.554 | 16.639 | 1.00 14.13 | C |
| ATOM | 45 | CG2 | ILE | A1009 | 18.619 | 3.696 | 16.642 | 1.00 13.71 | С |
| ATOM | 46 | CG1 | ILE | A1009 | 16.638 | 4.503 | 18.003 | 1.00 13.45 | С |
| ATOM | 47 | CD1 | ILE | A1009 | 16.175 | 3.134 | 18.434 | 1.00 15.16 | С |
| MOTA | 48 | С | ILE | A1009 | 16.318 | 6.799 | 16.257 | 1.00 14.09 | С |
| ATOM | 49 | 0 | ILE | A1009 | 16.033 | 7.589 | 17.165 | 1.00 12.83 | 0 |
| ATOM | 50 | N | ASP | A1010 | 15.491 | 6.537 | 15.232 | 1.00 14.68 | N |
| ATOM | 51 | CA | ASP | A1010 | 14.161 | 7.167 | 15.101 | 1.00 16.24 | С |
| ATOM | 52 | CB | ASP | A1010 | 14.287 | 8.580 | 14.496 | 1.00 17.11 | С |
| ATOM | 53 | CG | ASP | A1010 | 12.944 | 9.328 | 14.428 | 1.00 19.40 | С |
| ATOM | 54 | OD1 | ASP | A1010 | 12.265 | 9.295 | 13.369 | 1.00 19.82 | 0 |
| ATOM | 55 | OD2 | ASP | A1010 | 12.563 | 9.948 | 15.446 | 1.00 19.26 | 0 |
| MOTA | 56 | С | ASP | A1010 | 13.193 | 6.348 | 14.230 | 1.00 16.72 | С |
| ATOM | 57 | 0 | ASP | A1010 | 13.618 | 5.693 | 13.276 | 1.00 16.89 | 0 |
| ATOM | 58 | N | ILE | A1011 | 11.900 | 6.387 | 14.570 | 1.00 17.01 | N |
| MOTA | 59 | CA | ILE | A1011 | 10.850 | 5.706 | 13.796 | 1.00 17.33 | С |
| ATOM | 60 | CB | ILE | A1011 | 10.410 | 4.353 | 14.447 | 1.00 18.10 | С |
| MOTA | 61 | CG2 | ILE | A1011 | 9.963 | 4.570 | 15.898 | 1.00 17.28 | С |
| ATOM | 62 | CG1 | ILE | A1011 | 9.297 | 3.717 | 13.601 | 1.00 18.21 | С |
| ATOM | 63 | CD1 | ILE | A1011 | 8.852 | 2.338 | 14.083 | 1.00 20.73 | С |
| ATOM | 64 | С | ILE | A1011 | 9.648 | 6.664 | 13.679 | 1.00 18.00 | С |
| ATOM | 65 | 0 | ILE | A1011 | 9.262 | 7.298 | 14.663 | 1.00 16.80 | 0 |
| ATOM | 66 | N | GLU | A1012 | 9.060 | 6.760 | 12.481 | 1.00 18.22 | N |
| ATOM | 67 | CA | | A1012 | 7.951 | 7.690 | 12.220 | 1.00 19.38 | С |
| ATOM | 68 | CB | GLU | A1012 | 8.537 | 8.972 | 11.609 | 1.00 20.91 | С |
| ATOM | 69 | CG | GLU | A1012 | 7.537 | 10.036 | 11.186 | 1.00 23.69 | С |
| MOTA | 70 | CD | | A1012 | 7.065 | | 12.336 | 1.00 24.81 | C |
| MOTA | 71 | | | A1012 | 7.432 | 10.632 | 13.499 | 1.00 24.64 | 0 |
| MOTA | 72 | | | A1012 | 6.318 | | 12.070 | 1.00 27.04 | 0 |
| ATOM | 73 | С | | A1012 | 6.845 | | 11.293 | 1.00 19.45 | С |
| ATOM | 74 | ō | | A1012 | 7.119 | | 10.358 | 1.00 17.84 | 0 |
| ATOM | 75 | N | | A1013 | 5.599 | | 11.557 | 1.00 20.13 | N |
| ATOM | 76 | CA | | A1013 | 4.456 | | 10.735 | 1.00 21.62 | . C |
| ATOM | 77 | CB | | A1013 | 3.178 | | | 1.00 24.29 | C |
| | | | | | | | | | |

| | | | | | • | | | | | |
|------|-----|-----|------|---------|----------------|------------------|----------------|--------------------------|---|-----|
| ATOM | 78 | CG | GLU | A1013 | 1.916 | 6.753 | 10.845 | 1.00 28.34 | | C |
| ATOM | 79 | CD | | A1013 | 0.710 | 6.656 | 11.766 | 1.00 30.69 | | C |
| MOTA | 80 | OE1 | GLU | A1013 | -0.400 | 6.361 | 11.267 | 1.00 33.13 | | 0 |
| MOTA | 81 | OE2 | GLU | A1013 | 0.871 | 6.872 | 12.990 | 1.00 33.49 | : | 0 |
| ATOM | 82 | С | GLU | A1013 | 4.302 | 8.061 | 9.521 | 1.00 21.59 | · | C |
| ATOM | 83 | 0 | GLU | A1013 | 4.247 | 9.280 | 9.682 | 1.00 20.05 | | 0 |
| ATOM | 84 | N | LEU | A1014 | 4.223 | 7.493 | 8.316 | 1.00 21.61 | | N |
| ATOM | 85 | CA | LEU | A1014 | 4.104 | 8.288 | 7.087 | 1.00 22.02 | | С |
| ATOM | 86 | CB | LEU | A1014 | 4.191 | 7.365 | 5.857 | 1.00 23.16 | | С |
| ATOM | 87 | CG | LEU | A1014 | 5.502 | 6.571 | 5.745 | 1.00 24.38 | | С |
| ATOM | 88 | CD1 | LEU | A1014 | 5.454 | 5.622 | 4.551 | 1.00 25.08 | | С |
| ATOM | 89 | CD2 | LEU | A1014 | 6.667 | 7.538 | 5.604 | 1.00 25.38 | | С |
| ATOM | 90 | С | LEU | A1014 | 2.841 | 9.158 | 7.006 | 1.00 22.02 | | C |
| ATOM | 91 | 0 | LEU | A1014 | 2.867 | 10.240 | 6.419 | 1.00 21.55 | | 0 |
| MOTA | 92 | N | ALA | A1015 | 1.742 | 8.691 | 7.593 | 1.00 22.06 | | N |
| ATOM | 93 | CA | ALA | A1015 | 0.488 | 9.452 | 7.595 | 1.00 22.62 | | С |
| MOTA | 94 | CB | ALA | A1015 | -0.605 | 8.656 | 8.299 | 1.00 22.21 | | C |
| ATOM | 95 | C | ALA | A1015 | 0.644 | 10.817 | 8.274 | 1.00 22.87 | | С |
| ATOM | 96 | 0 | ALA | A1015 | 0.005 | 11.796 | 7.875 | 1.00 23.00 | | 0 |
| ATOM | 97 | N | SER | A1016 | 1.482 | 10.876 | 9.307 | 1.00 23.27 | | N |
| ATOM | 98 | CA | SER | A1016 | 1.716 | 12.123 | 10.034 | 1.00 23.77 | | С |
| ATOM | 99 | CB | SER | A1016 | 2.535 | 11.860 | 11.305 | 1.00 24.30 | | С |
| ATOM | 100 | OG | SER | A1016 | 1.890 | 10.919 | 12.145 | 1.00 26.09 | | 0 |
| ATOM | 101 | С | SER | A1016 | 2.443 | 13.146 | 9.162 | 1.00 23.41 | | С |
| ATOM | 102 | 0 | SER | A1016 | 2.173 | 14.348 | 9.249 | 1.00 23.19 | - | 0 |
| MOTA | 103 | N | ILE | A1017 | 3.378 | 12.673 | 8.340 | 1.00 23.05 | | N |
| ATOM | 104 | CA | ILE | A1017 | 4.118 | 13.566 | 7.450 | 1.00 22.92 | | С |
| MOTA | 105 | CB | ILE | A1017 | 5.355 | 12.860 | 6.838 | 1.00 23.00 | | С |
| ATOM | 106 | CG2 | ILE | A1017 | 6.107 | 13.823 | 5.918 | 1.00 23.26 | | С |
| ATOM | 107 | CG1 | ILE | A1017 | 6.289 | 12.365 | 7.951 | 1.00 23.63 | | C |
| ATOM | 108 | CD1 | ILE | A1017 | 6.896 | 13.467 | 8.810 | 1.00 22.84 | | , C |
| MOTA | 109 | C | ILE | A1017 | 3.204 | 14.053 | 6.308 | 1.00 23.44 | | С |
| MOTA | 110 | 0 | ILE | A1017 | 3.276 | .15.218 | 5.896 | 1.00 23.11 | | 0 |
| ATOM | 111 | N | GLU | A1018 | 2.341 | 13.170 | 5.805 | 1.00 22.98 | | N |
| ATOM | 112 | CA | | A1018 | 1.443 | 13.549 | 4.714 | 1.00 24.09 | | C |
| ATOM | 113 | СВ | GLU | A1018 | 0.729 | 12.306 | 4.147 | 1.00 25.23 | | С |
| ATOM | 114 | CG | GLU | A1018 | -0.252 | 12.592 | 2.997 | 1.00 27.75 | | C |
| ATOM | 115 | CD | | A1018 | -0.632 | 11.345 | 2.190 | 1.00 29.64 | | С |
| ATOM | 116 | | | A1018 | -0.807 | 10.255 | 2.783 | 1.00 30.50 | | 0 |
| MOTA | 117 | OE2 | | A1018 | -0.771 | 11.459 | 0.952 | 1.00 30.61 | | . 0 |
| ATOM | 118 | С | | A1018 | 0.427 | 14.612 | 5.150 | 1.00 24.15 | | . C |
| MOTA | 119 | 0 | | A1018 | 0.142 | 15.550 | 4.395 | 1.00 23.68 | | И |
| MOTA | 120 | N | | A1019 | -0.103 | 14.481 | 6.367 | 1.00 23.86 | | C |
| MOTA | 121 | CA | | A1019 | -1.078 | 15.445 | 6.879 | 1.00 24.87 | | C |
| ATOM | 122 | СВ | | A1019 | -1.641 | 14.993 | 8.234 | 1.00 24.60 1.00 26.37 | | 0 |
| MOTA | 123 | OG | | R A1019 | -2.387 | 13.794 | 8.120 | | | C |
| MOTA | 124 | С | | R A1019 | -0.450 | 16.824 | 7.045 | 1.00 25.06 | | o |
| ATOM | 125 | 0 | | R A1019 | -1.077 | 17.836 | 6.741 7.525 | 1.00 25.39 1.00 25.98 | | N |
| ATOM | 126 | N | | A1020 | 0.790 | 16.856 | | 1.00 25.36 | | C |
| ATOM | 127 | CA | | A A1020 | 1.508 | 18.112 | 7.748 | 1.00 26.48 | | Č |
| ATOM | 128 | CB | | A A1020 | 2.869 | 17.829 | 8.399 | | | c |
| ATOM | 129 | C | | A A1020 | 1.695 | 18.909 | 6.460 | 1.00 26.83 1.00 26.25 | | 0 |
| MOTA | 130 | 0 | | A A1020 | 1.589 | 20.138 | 6.463 | 1.00 20.23 | | N |
| ATOM | 131 | N | | A1021 | 1.974 | 18.210 18.855 | 5.364 4.064 | 1.00 27.31 | | C |
| ATOM | 132 | CA | | L A1021 | 2.166 2.767 | 17.868 | 3.029 | | | c |
| ATOM | 133 | CB | | L A1021 | | | 1.639 | | | č |
| MOTA | 134 | CG. | T AV | L A1021 | 2.801 | 18.510 | 1.039 | 1.00 20.03 | | |

| ATOM | 135 | CG2 | VAL | A1021 | | 4.176 | 17.461 | 3.457 | 1.00 28.09 | С |
|--------------|------------|----------|-----|----------------|---|----------------|------------------|----------------|--------------------------|--------|
| ATOM | 136 | С | VAL | A1021 | | 0.845 | 19.396 | 3.512 | 1.00 30.16 | С |
| ATOM | 137 | | | A1021 | | 0.775 | 20.541 | 3.054 | 1.00 29.31 | . 0 |
| ATOM | 138 | N | THR | A1022 | | -0.195 | 18.565 | 3.557 | 1.00 31.76 | N |
| ATOM | 139 | | | A1022 | | -1.515 | 18.951 | 3.057 | 1.00 33.81 . | С |
| ATOM | 140 | | | A1022 | | -2.541 | 17.798 | 3.230 | 1.00 33.53 | C |
| ATOM | 141 | | | A1022 | | -2.119 | 16.663 | 2.466 | 1.00 33.79 | 0 |
| ATOM | 142 | | | A1022 | | -3.926 | 18.224 | 2.749 | 1.00 33.72 | . С |
| ATOM | 143 | С | THR | A1022 | | -2.032 | 20.183 | 3.790 | 1.00 34.97 | · C |
| ATOM | 144 | 0 | | A1022 | | -2.802 | 20.968 | 3.237 | 1.00 36.01 | 0 |
| ATOM | 145 | N | ARG | A1023 | | -1.585 | 20.346 | 5.029 | 36.61, 1.00 | N |
| MOTA | 146 | CA | ARG | A1023 | | -1.988 | 21.462 | 5.876 | 1.00 38.01 | C |
| ATOM | 147 | CB | ARG | A1023 | | -1.371 | 21.297 | 7.267 | 1.00 38.96 | С |
| ATOM | 148 | CG | ARG | A1023 | | -2.284 | 21.702 | 8.409 | 1.00 40.44 | С |
| ATOM | 149 | CD | ARG | A1023 | | -2.443 | 20.556 | 9.393 | 1.00 41.63 | С |
| ATOM | 150 | NE | ARG | A1023 | | -1.184 | 20.219 | 10.053 | 1.00 42.83 | N |
| MOTA | 151 | CZ | ARG | A1023 | | -1.000 | 19.134 | 10.800 | 1.00 43.45 | С |
| ATOM | 152 | NH1 | ARG | A1023 | | -1.997 | 18.277 | 10.981 | 1.00 43.85 | N |
| ATOM | 153 | NH2 | ARG | A1023 | | 0.178 | 18.906 | 11.367 | 1.00 43.30 | N |
| MOTA | 154 | С | ARG | A1023 | | -1.603 | 22.825 | 5.302 | 1.00 38.55 | С |
| ATOM | 155 | 0 | ARG | A1023 | | -2.143 | 23.850 | 5.722 | 1.00 38.81 | 0 |
| ATOM | 156 | N | HIS | A1024 | | -0.663 | 22.842 | 4.359 | 1.00 38.91 | N |
| MOTA | 157 | CA | HIS | A1024 | | -0.244 | 24.096 | 3.733 | 1.00 38.99 | С |
| ATOM | 158 | CB | HIS | A1024 | | -1.432 | 24.654 | 2.935 | 1.00 40.09 | С |
| ATOM | 159 | CG | HIS | A1024 | | -1.184 | 25.993 | 2.315 | 1.00 41.43 | C |
| ATOM | 160 | CD2 | HIS | A1024 | | -1.936 | 27.119 | 2.304 | 1.00 41.88 | С |
| MOTA | 161 | ND1 | HIS | A1024 | | -0.058 | 26.276 | 1.573 | 1.00 41.78 | N |
| ATOM | 162 | CE1 | HIS | A1024 | | -0.126 | 27.519 | 1.131 | 1.00 42.17 | С |
| ATOM | 163 | NE2 | HIS | A1024 | | -1.257 | 28.053 | 1.560 | 1.00 42.70 | N |
| MOTA | 164 | С | HIS | A1024 | | 0.245 | 25.107 | 4.782 | 1.00 38.60 | С |
| MOTA | 165 | 0 | HIS | A1024 | | -0.251 | 26.236 | 4.857 | 1.00 38.61 | 0 |
| ATOM | 166 | N | GLU | A1025 | | 1.234 | 24.696 | 5.575 | 1.00 37.69 | N |
| ATOM | 167 | CA | | A1025 | | 1.784 | 25.533 | 6.643 | 1.00 36.89 | C |
| MOTA | 168 | CB | | A1025 | - | 1.545 | 24.854 | 7.995 | 1.00 37.94 | C |
| MOTA | 169 | CG | | A1025 | | 2.255 | 23.508 | 8.126 | 1.00 39.13 | C C |
| ATOM | 170 | CD | | A1025 | | 2.003 | 22.828 | 9.459 | 1.00 40.28 | 0 |
| MOTA | 171 | | | A1025 | | 0.853 | 22.405 | 9.709 | 1.00 41.24 | 0 |
| ATOM | 172 | | | A1025 | | 2.959 | 22.716 | 10.258 | 1.00 40.84 | C |
| ATOM | 173 | С | | A1025 | | 3.280 | 25.856 | 6.518 | 1.00 35.45 1.00 35.71 | 0 |
| ATOM | 174 | 0 | | A1025 | | 3.857 | 26.466 | 7.424 5.420 | 1.00 33.71 | N |
| ATOM | 175 | N | | A1026 | | 3.906 5.324 | 25.441 25.708 | 5.220 | 1.00 30.99 | c |
| ATOM | 176 | CA | | A1026 A1026 | | 6.265 | 24.668 | 5.819 | 1.00 29.44 | Č |
| ATOM | 177 | С | | A1026 | | 7.448 | 24.943 | 6.040 | 1.00 28.80 | 0 |
| ATOM | 178 179 | O N | | A1028 | | 5.743 | 23.470 | 6.073 | 1.00 27.49 | N |
| MOTA | | - | | A1027 | | 6.524 | 22.378 | 6.657 | 1.00 26.42 | C |
| ATOM | 180 | CA CB | | E A1027 | | 5.618 | 21.149 | 6.830 | 1.00 26.50 | C |
| ATOM | 181 182 | CG | | E A1027 | | 6.272 | 19.995 | 7.541 | 1.00 26.07 | C |
| MOTA | 183 | | | E A1027 | | 6.650 | 20.103 | 8.876 | 1.00 25.99 | C |
| ATOM | 184 | | | E A1027 | | 6.499 | 18.790 | 6.873 | 1.00 26.17 | С |
| MOTA MOTA | 185 | | | E A1027 | | 7.243 | 19.028 | 9.541 | 1.00 26.70 | C |
| | 186 | | | E A1027 | | 7.091 | 17.711 | 7.527 | | С |
| MOTA MOTA | 187 | CEZ | | E A1027 | | 7.465 | | 8.863 | | C |
| ATOM | 188 | C | | E A1027 | | 7.776 | | 5.852 | | C |
| ATOM | 189 | 0 | | E A1027 | | 8.892 | | 6.377 | | 0 |
| ATOM | 190 | N | | A A1028 | | 7.598 | | 4.579 | | N |
| MOTA | 191 | CA | | A A1028 | | 8.726 | | 3.737 | | C |
| 0 | | | | | | | | | | |

| n moss | 100 | CD. | א ז א | A1028 | 8.232 | 20.919 | 2.333 | 1.00 24.87 | С |
|--------|-----|-----|-------|---------|--------|--------|----------------|------------|-----|
| ATOM | 192 | | | A1028 | 9.824 | 22.325 | 3.661 | 1.00 25.07 | С |
| ATOM | 193 | _ | | | 11.018 | 22.009 | 3.685 | 1.00 24.02 | 0 |
| ATOM | 194 | | | A1028 | 9.417 | 23.587 | 3.571 | 1.00 25.80 | N |
| MOTA | 195 | | | A1029 | | 24.695 | 3.488 | 1.00 26.80 | Ċ |
| MOTA | 196 | | | A1029 | 10.364 | | 3.222 | 1.00 28.18 | Ċ |
| MOTA | 197 | | | A1029 | 9.598 | 26.000 | | 1.00 30.30 | č |
| MOTA | 198 | | | A1029 | 10.449 | 27.200 | 2.800 | 1.00 30.30 | Č |
| MOTA | 199 | | | A1029 | 11.251 | 27.769 | 3.958 | | C |
| MOTA | 200 | | | A1029 | 11.799 | 29.151 | 3.636 | 1.00 33.23 | N |
| MOTA | 201 | NZ | LYS | A1029 | 10.702 | 30.153 | 3.506 | 1.00 34.55 | |
| MOTA | 202 | C | | A1029 | 11.197 | 24.806 | 4.771 | 1.00 26.54 | C |
| MOTA | 203 | 0 | LYS | A1029 | 12.344 | 25.244 | 4.738 | 1.00 26.39 | 0 |
| ATOM | 204 | N | ARG | A1030 | 10.624 | 24.394 | 5.897 | 1.00 26.43 | N |
| ATOM | 205 | CA | ARG | A1030 | 11.327 | 24.464 | | 1.00 26.50 | C |
| ATOM | 206 | CB | ARG | A1030 | 10.312 | 24.485 | 8.334 | 1.00 27.57 | С |
| ATOM | 207 | CG | | A1030 | 10.945 | 24.487 | 9.727 | 1.00 30.51 | С |
| ATOM | 208 | CD | ARG | A1030 | 9.933 | 24.858 | 10.820 | 1.00 31.96 | С |
| ATOM | 209 | NE | ARG | A1030 | 8.887 | 23.851 | 11.008 | 1.00 32.84 | N |
| ATOM | 210 | CZ | | A1030 | 9.033 | 22.740 | 11.723 | 1.00 33.04 | С |
| ATOM | 211 | | | A1030 | 10.184 | 22.482 | 12.327 | 1.00 33.30 | N |
| ATOM | 212 | | | A1030 | 8.028 | 21.884 | 11.836 | 1.00 33.60 | N |
| ATOM | 213 | C | | A1030 | 12.325 | 23.327 | 7.407 | 1.00 25.55 | С |
| | 214 | 0 | | A1030 | 13.402 | 23.539 | 7.976 | 1.00 25.72 | 0 |
| ATOM | | | | A1031 | 11.967 | 22.130 | 6.952 | 1.00 24.16 | N |
| ATOM | 215 | N | | A1031 | 12.795 | 20.934 | 7.134 | 1.00 23.09 | С |
| ATOM | 216 | CA | | A1031 | 11.903 | 19.655 | 7.150 | 1.00 23.53 | С |
| MOTA | 217 | CB | | | 12.765 | 18.398 | 7.339 | 1.00 23.93 | С |
| ATOM | 218 | | | A1031 | 10.874 | 19.754 | 8.258 | 1.00 22.96 | С |
| ATOM | 219 | | | A1031 | 13.932 | 20.684 | 6.134 | 1.00 22.57 | C |
| MOTA | 220 | С | | A1031 | | | 6.504 | 1.00 22.31 | Ō |
| MOTA | 221 | 0 | | A1031 | 14.952 | 20.094 | 4.887 | 1.00 21.47 | N |
| MOTA | 222 | N | | A1032 | 13.765 | 21.127 | | 1.00 21.77 | c |
| MOTA | 223 | CA | | A1032 | 14.764 | 20.888 | 3.830 | 1.00 21.78 | Ċ |
| ATOM | 224 | CB | | A1032 | 14.062 | 20.277 | 2.607 | 1.00 21.33 | C |
| MOTA | 225 | CG | | A1032 | 13.126 | 19.073 | 2.773 1.428 | 1.00 20.73 | C |
| MOTA | 226 | | | A1032 | 12.446 | 18.779 | | 1.00 21.22 | C |
| ATOM | 227 | | | A1032 | 13.912 | 17.851 | 3.249 | 1.00 20.00 | ç. |
| ATOM | 228 | С | | A1032 | 15.565 | 22.107 | 3.355 3.375 | 1.00 22.39 | ő |
| ATOM | 229 | 0 | | A1032 | 15.061 | 23.233 | | | N |
| ATOM | 230 | N | | A1033 | 16.806 | 21.875 | 2.917 | 1.00 23.26 | Č |
| MOTA | 231 | CA | | R A1033 | 17.661 | 22.951 | 2.394 | 1.00 24.31 | c |
| ATOM | 232 | CB | | R A1033 | 19.171 | 22.577 | 2.366 | 1.00 24.32 | 0 |
| ATOM | 233 | | | R A1033 | 19.380 | 21.472 | 1.473 | 1.00 24.43 | C |
| ATOM | 234 | CG2 | | R A1033 | 19.671 | 22.217 | 3.756 | 1.00 23.93 | C |
| ATOM | 235 | С | | R A1033 | 17.255 | 23.215 | 0.945 | 1.00 25.20 | 0 |
| MOTA | 236 | 0 | | R A1033 | 16.343 | | 0.426 | 1.00 24.87 | |
| ATOM | 237 | N | AL | A A1034 | 17.937 | | 0.297 | 1.00 25.70 | N |
| MOTA | 238 | CA | ALA | A A1034 | 17.650 | | -1.100 | 1.00 26.57 | C |
| ATOM | 239 | CB | AL | A A1034 | 18.485 | | -1.548 | | C |
| ATOM | 240 | С | AL | A A1034 | 17.943 | | -1.997 | | C |
| MOTA | 241 | 0 | AL | A A1034 | 17.115 | 22.896 | -2.829 | | 0 |
| ATOM | 242 | N | | J A1035 | 19.122 | 22.672 | -1.831 | | N |
| ATOM | 243 | | | U A1035 | 19.513 | | -2.623 | | С |
| ATOM | 244 | СВ | | U A1035 | 20.943 | | | | С |
| ATOM | 245 | | | U A1035 | 22.137 | | | 1.00 28.71 | С |
| ATOM | 246 | | | U A1035 | 23.388 | | | 1.00 28.34 | C |
| ATOM | 247 | | | U A1035 | 22.348 | | | | С |
| ATOM | 248 | | | U A1035 | 18.549 | | | 1.00 26.73 | , c |
| | 2.0 | _ | | | | | | | |

| ATOM | 249 | 0 | LEU | A1035 | 18.124 | 19.679 | -3.369 | 1.00 | 26.11 | 0 | |
|------|-----|-----|-----|---------|--------|--------|--------|------|-------|---|---|
| ATOM | 250 | N | GLU | A1036 | 18.209 | 20.048 | -1.151 | 1.00 | 26.36 | N | |
| MOTA | 251 | CA | GLU | A1036 | 17.285 | 18.958 | -0.852 | 1.00 | 26.00 | С | |
| ATOM | 252 | СВ | GLU | A1036 | 17.119 | 18.801 | 0.675 | 1.00 | 24.96 | С | |
| ATOM | 253 | | GLU | A1036 | 18.307 | 18.111 | 1.367 | 1.00 | 22.07 | С | |
| ATOM | 254 | CD | GLU | A1036 | 18.254 | 18.150 | 2.900 | 1.00 | 22.03 | C | : |
| ATOM | 255 | | | A1036 | 18.819 | 17.229 | 3.540 | 1.00 | 20.25 | 0 |) |
| ATOM | 256 | | | A1036 | 17.671 | 19.102 | 3.472 | 1.00 | 19.80 | 0 | J |
| ATOM | 257 | С | | A1036 | 15.934 | 19.228 | -1.526 | 1.00 | 27.44 | C | : |
| ATOM | 258 | Õ | | A1036 | 15.296 | 18.314 | -2.060 | 1.00 | 26.45 | 0 |) |
| ATOM | 259 | N | | A1037 | 15.514 | 20.493 | -1.525 | | 28.51 | N | 1 |
| ATOM | 260 | CA | | A1037 | 14.242 | 20.888 | -2.132 | 1.00 | 30.20 | C | ; |
| ATOM | 261 | CB | | A1037 | 13.979 | 22.377 | -1.877 | 1.00 | 31.18 | C | : |
| ATOM | 262 | CG | | A1037 | 12.608 | 22.872 | -2.324 | 1.00 | 32.64 | C | |
| ATOM | 263 | SD | | A1037 | 11.236 | 22.231 | -1.342 | | 35.22 | S | |
| ATOM | 264 | CE | | A1037 | 9.873 | 22.344 | -2.511 | | 34.31 | C | |
| ATOM | 265 | C | | A1037 | 14.192 | 20.608 | -3.637 | | 30.82 | C | |
| ATOM | 266 | ō | | A1037 | 13.141 | 20.248 | -4.176 | | 31.12 | C | |
| ATOM | 267 | N | | A1038 | 15.320 | 20.780 | -4.317 | | 31.36 | N | J |
| ATOM | 268 | CA | | A1038 | 15.371 | 20.526 | -5.756 | | 31.95 | C | ; |
| ATOM | 269 | CB | | A1038 | 16.773 | 20.820 | -6.296 | | 33.04 | C | |
| ATOM | 270 | CG | | A1038 | 17.111 | 22.300 | -6.367 | | 35.12 | C | |
| ATOM | 271 | CD | | A1038 | 18.578 | 22.550 | -6.673 | | 36.56 | C | |
| ATOM | 272 | | | A1038 | 18.943 | 23.713 | -6.941 | | 37.89 | C | |
| ATOM | 273 | | | A1038 | 19.371 | 21.585 | -6.639 | | 37.49 | C | |
| ATOM | 274 | C | | A1038 | 14.988 | 19.080 | -6.072 | | 31.21 | (| |
| ATOM | 275 | 0 | | A1038 | 14.268 | 18.816 | -7.036 | | 30.88 | (|) |
| ATOM | 276 | Ŋ | | A1039 | 15.474 | 18.151 | -5.253 | | 29.97 | | N |
| ATOM | 277 | CA | | A1039 | 15.188 | 16.730 | -5.427 | | 28.84 | | 3 |
| ATOM | 278 | CB | | A1039 | 16.086 | 15.913 | -4.483 | | 29.69 | | 2 |
| ATOM | 279 | CG | | A1039 | 15.853 | 14.402 | -4.480 | | 31.09 | (| C |
| ATOM | 280 | CD | | A1039 | 16.329 | 13.727 | -5.758 | | 32.23 | (| C |
| MOTA | 281 | NE | | A1039 | 16.125 | 12.280 | -5.708 | | 33.37 | | N |
| ATOM | 282 | CZ | | A1039 | 16.076 | | -6.780 | | 33.30 | (| С |
| ATOM | 283 | | | A1039 | 16.222 | 12.007 | -7.992 | | 33.19 | 1 | N |
| ATOM | 284 | | | A1039 | 15.852 | 10.191 | -6.641 | | 32.92 | 1 | N |
| ATOM | 285 | C | | A1039 | 13.709 | 16.442 | -5.145 | 1.00 | 27.71 | (| С |
| ATOM | 286 | 0 | | A1039 | 13.059 | 15.705 | -5.887 | | 26.61 | (| 0 |
| ATOM | 287 | N | | A1040 | 13.189 | 17.041 | -4.076 | | 26.75 | 1 | N |
| ATOM | 288 | CA | | A1040 | 11.795 | 16.867 | -3.659 | 1.00 | 26.16 | | С |
| ATOM | 289 | СВ | | A1040 | 11.532 | 17.729 | -2.405 | 1.00 | 25.81 | | С |
| ATOM | 290 | CG | | A1040 | 10.111 | 17.665 | -1.886 | 1.00 | 25.91 | (| С |
| ATOM | 291 | | | A1040 | 9.615 | 16.508 | -1.292 | 1.00 | 25.16 | | С |
| ATOM | 292 | | | A1040 | 9.275 | 18.778 | -1.979 | 1.00 | 25.61 | | С |
| ATOM | 293 | CE1 | PHE | A1040 | 8.309 | 16.457 | -0.798 | 1.00 | 25.37 | | С |
| ATOM | 294 | CE2 | PHE | A1040 | 7.966 | 18.740 | -1.490 | 1.00 | 25.17 | | С |
| ATOM | 295 | CZ | | A1040 | 7.481 | 17.579 | -0.897 | 1.00 | 25.69 | | С |
| ATOM | 296 | С | | A1040 | 10.782 | 17.210 | -4.760 | 1.00 | 25.80 | | С |
| ATOM | 297 | 0 | PHE | A1040 | 9.835 | 16.460 | -4.990 | 1.00 | 25.42 | | 0 |
| ATOM | 298 | N | THR | A1041 | 10.984 | 18.332 | -5.443 | 1.00 | 25.73 | | N |
| MOTA | 299 | CA | THR | A1041 | 10.053 | 18.759 | -6.493 | | 2624 | | С |
| ATOM | 300 | СВ | | A1041 | 10.257 | 20.259 | -6.836 | 1.00 | 26.86 | | С |
| ATOM | 301 | | | A1041 | 11.634 | 20.507 | -7.154 | | 26.58 | | 0 |
| ATOM | 302 | CG2 | THE | A1041 | 9.849 | 21.130 | -5.656 | | 26.06 | | С |
| ATOM | 303 | С | THE | R A1041 | 10.066 | 17.948 | -7.800 | | 26.59 | | С |
| ATOM | 304 | 0 | | R A1041 | 9.149 | 18.071 | -8.620 | | 27.01 | | 0 |
| ATOM | 305 | N | SEF | R A1042 | 11.080 | 17.111 | -7.996 | 1.00 | 26.31 | | N |
| | | | | | | | | | | | |

| ATC | M | 306 | CA | SER | A1042 | 11.158 | 16.305 | -9.222 | 1.00 26.03 | С |
|-----|-----|-----|-----------|-----|---------|----------------|------------------|--------------------|------------|-----|
| ATC | | 307 | СВ | | A1042 | 12.618 | 16.106 | -9.631 | 1.00 26.30 | С |
| ATC | | 308 | OG | | A1042 | 13.287 | 15.231 | -8.737 | 1.00 27.19 | 0 |
| ATC | | 309 | C | | A1042 | 10.488 | | -9.082 | 1.00 25.97 | С |
| ATC | | 310 | Õ | | A1042 | 10.354 | | -10.063 | 1.00 25.27 | 0 |
| ATO | | 311 | N | | A1043 | 10.064 | 14.599 | -7.865 | 1.00 25.25 | N |
| ATC | | 312 | CA | | A1043 | 9.431 | 13.310 | -7.601 | 1.00 25.51 | С |
| | | 313 | CB | | A1043 | 9.906 | 12.765 | -6.245 | 1.00 24.11 | Ċ |
| ATC | | | | | A1043 | 11.425 | 12.571 | -6.118 | 1.00 24.06 | Ċ |
| ATC | | 314 | CG CD1 | | | 11.768 | 12.080 | -4.715 | 1.00 22.60 | Ċ |
| ATC | | 315 | | | A1043 | | | -7.164 | 1.00 23.86 | č |
| ATO | | 316 | | | A1043 | 11.914 | 11.571 13.389 | -7.634 | 1.00 25.82 | c |
| ATO | | 317 | С | | A1043 | 7.907 | | -7.575 | 1.00 26.42 | ő |
| ATC | | 318 | 0 | | A1043 | 7.333 | 14.475 | -7.723 | 1.00 26.42 | Ŋ |
| ATO | | 319 | N | | A1044 | 7.256 | 12.233 | | | C |
| ATO | | 320 | CA | | A1044 | 5.802 | 12.184 | -7.785 | 1.00 27.60 | C |
| ATO | | 321 | CB | | A1044 | 5.361 | 11.803 | -9.200 | 1.00 29.18 | |
| ATO | MC | 322 | CG | | A1044 | 5.705 | 10.369 | -9.562 | 1.00 31.06 | C |
| AT(| MC | 323 | CD | | A1044 | 5.359 | | -10.999 | 1.00 32.81 | C |
| ATO | MC | 324 | CE | LYS | A1044 | 5.572 | | -11.282 | 1.00 33.54 | C |
| ATO | MC | 325 | ΝZ | LYS | A1044 | 4.702 | | -10.419 | 1.00 34.84 | N |
| AT | MO | 326 | С | LYS | A1044 | 5.159 | 11.211 | | 1.00 27.94 | C |
| AT | OM | 327 | 0 | LYS | A1044 | 5.774 | 10.227 | -6.367 | 1.00 27.61 | 0 |
| AT | OM | 328 | N | GLY | A1045 | 3.904 | 11.500 | -6.464 | 1.00 27.68 | И |
| AT | OM | 329 | CA | GLY | A1045 | 3.124 | 10.671 | - 5.562 | 1.00 28.74 | С |
| AT | | 330 | С | GLY | A1045 | 3.741 | 10.224 | -4.252 | 1.00 28.99 | С |
| AT | | 331 | 0 | GLY | A1045 | 4.282 | 11.024 | -3.487 | 1.00 29.00 | 0 |
| AT | | 332 | N | | A1046 | 3.643 | 8.925 | -3.998 | 1.00 29.30 | N |
| AT | | 333 | CA | | A1046 | 4.155 | 8.320 | -2.776 | 1.00 30.48 | C |
| AT | | 334 | CB | | A1046 | 3.790 | 6.833 | -2.754 | 1.00 32.57 | C |
| AT | | 335 | CG | | A1046 | 3.044 | 6.390 | -1.513 | 1.00 35.84 | С |
| AT | | 336 | CD | | A1046 | 2.680 | 4.922 | | 1.00 38.51 | C |
| AT | | 337 | NE | | A1046 | 2.023 | 4.445 | | 1.00 41.12 | N |
| | OM | 338 | CZ | | A1046 | 1.613 | 3.194 | | 1.00 42.33 | С |
| | OM | 339 | | | A1046 | 1.024 | 2.842 | | 1.00 42.60 | N |
| | OM | 340 | | | A1046 | 1.793 | 2.292 | | 1.00 43.25 | N |
| | OM | 341 | C | | A1046 | 5.663 | 8.479 | | 1.00 29.60 | С |
| | OM | 342 | Ö | | A1046 | 6.128 | | | 1.00 28.95 | 0 |
| | 'OM | 343 | N | | A1047 | 6.423 | 8.375 | | 1.00 28.70 | N |
| | 'OM | 344 | CA | | A1047 | 7.875 | 8.495 | | 1.00 28.01 | С |
| | 'OM | 345 | CB | | A1047 | 8.512 | | | 1.00 29.65 | С |
| | OM | 346 | CG | | A1047 | 9.566 | | | 1.00 32.09 | С |
| | | 347 | | | A1047 | 9.831 | | | 1.00 34.53 | С |
| | MO: | | CD | | A1047 | 8.601 | | | 1.00 36.57 | N |
| | MOY | 348 | NE | | | 8.548 | | | 1.00 37.35 | Ċ |
| | MOT | 349 | CZ | | A1047 | | | | 1.00 37.33 | N |
| | MO | 350 | | | A1047 | 7.373 9.663 | | | 1.00 38.02 | N |
| | MOT | 351 | | | A1047 | | | | 1.00 26.86 | C |
| | MOT | 352 | C | | A1047 | 8.288 | | | 1.00 25.61 | Õ |
| | MOT | 353 | 0 | | A1047 | 9.309 | | | 1.00 25.01 | N |
| | MO | 354 | N | | A1048 | 7.481 | | | | c |
| | MOT | 355 | CA | | A1048 | 7.739 | | | | c |
| | MOT | 356 | CB | | A1048 | 6.733 | | | | , c |
| | MOT | 357 | CG | | A1048 | 7.138 | | | | . c |
| | MOT | 358 | CD | | A1048 | . 6.221 | | | | 0 |
| | MOT | 359 | | | A1048 | 6.617 | | | | |
| | TOM | 360 | | | A1048 | 4.994 | | | | N |
| | TOM | 361 | С | | 1 A1048 | 7.632 | | | | C |
| A. | MOT | 362 | 0 | GLN | N A1048 | 8.463 | 13.110 | 0 -0.935 | 1.00 23.01 | 0 |
| | | | | | | | | | | |

| ATOM | 363 | N | ILE . | A1049 | 6.615 | 11.830 | -0.949 | 1.00 22.49 | N |
|--------------|------------|----------|-------|----------------|------------------|------------------|----------------|--------------------------|--------|
| ATOM | 364 | CA | ILE . | A1049 | 6.423 | 11.919 | 0.504 | 1.00 22.00 | C |
| ATOM | 365 | CB | ILE . | A1049 | 5.011 | 11.414 | 0.916 | 1.00 23.38 | C |
| ATOM | 366 | CG2 | ILE . | A1049 | 4.810 | 11.564 | 2.421 | 1.00 23.48 | С |
| ATOM | 367 | CG1 | ILE | A1049 | 3.928 | 12.197 | 0.161 | 1.00 24.39 | C |
| MOTA | 368 | CD1 | ILE | A1049 | 3.923 | 13.695 | 0.424 | 1.00 25.65 | C |
| ATOM | 369 | С | ILE | A1049 | 7.496 | 11.118 | 1.274 | 1.00 21.25 | C |
| ATOM | 370 | | | A1049 | 7.940 | 11.537 | 2.347 | 1.00 19.66 | 0 N |
| ATOM | 371 | | | A1050 | 7.913 | 9.975 | 0.724 | 1.00 20.69 | C |
| ATOM | 372 | | | A1050 | 8.939 | 9.146 | 1.372 | 1.00 20.67 1.00 22.03 | . c |
| ATOM | 373 | | | A1050 | 9.093 | 7.794 | 0.650 | 1.00 22.03 | . C |
| MOTA | 374 | | | A1050 | 10.362 | 7.017 | 1.051 2.520 | 1.00 23.09 | Ċ |
| MOTA | 375 | | | A1050 | 10.385 | 6.625 | 3.095 | 1.00 23.91 | Ö |
| ATOM | 376 | | | A1050 | 11.498 | 6.519 | 3.097 | 1.00 25.89 | 0 |
| ATOM | 377 | | | A1050 | 9.292 | 6.409 9.851 | 1.430 | 1.00 23.03 | č |
| ATOM | 378 | С | | A1050 | 10.298 11.073 | 9.634 | 2.367 | 1.00 19.12 | Ö |
| ATOM | 379 | 0 | | A1050 | 10.604 | 10.680 | 0.431 | 1.00 18.43 | N |
| ATOM | 380 | N | | A1051 | 11.878 | 11.400 | 0.435 | 1.00 17.86 | C |
| ATOM | 381 | CA | | A1051 | 12.110 | 12.129 | -0.902 | 1.00 18.12 | Ċ |
| ATOM | 382 | CB | | A1051 | 13.379 | 12.123 | -0.932 | 1.00 17.88 | Ċ |
| MOTA | 383 | CG | | A1051 A1051 | 13.379 | 14.307 | -0.518 | 1.00 17.74 | C |
| ATOM | 384 | | | A1051 | 14.547 | 15.076 | -0.516 | 1.00 17.82 | С |
| ATOM | 385 386 | | | A1051 | 14.592 | 12.419 | -1.345 | 1.00 17.56 | С |
| ATOM ATOM | 387 | | | A1051 | 15.770 | 13.176 | -1.344 | 1.00 18.21 | С |
| ATOM | 388 | CZ | | A1051 | 15.740 | 14.501 | -0.929 | 1.00 18.16 | С |
| ATOM | 389 | OH | | A1051 | 16.908 | 15.237 | -0.923 | 1.00 18.28 | 0 |
| ATOM | 390 | C | | A1051 | 11.915 | 12.409 | 1.590 | 1.00 17.91 | С |
| ATOM | 391 | Ö | | A1051 | 12.927 | 12.525 | 2.290 | 1.00 16.53 | 0 |
| ATOM | 392 | N | | A1052 | 10.810 | 13.137 | 1.778 | 1.00 17.38 | N |
| ATOM | 393 | CA | | A1052 | 10.709 | 14.131 | 2.851 | 1.00 17.07 | С |
| ATOM | 394 | СВ | LEU | A1052 | 9.392 | 14.917 | 2.731 | 1.00 17.53 | С |
| MOTA | 395 | CG | LEU | A1052 | 8.985 | 15.844 | 3.890 | 1.00 17.80 | С |
| ATOM | 396 | CD1 | LEU | A1052 | 10.096 | 16.844 | 4.191 | 1.00 18.32 | C |
| ATOM | 397 | CD2 | LEU | A1052 | 7.693 | 16.573 | 3.524 | 1.00 17.67 | C |
| MOTA | 398 | С | LEU | A1052 | 10.784 | 13.448 | 4.219 | 1.00 16.62 | C |
| MOTA | 399 | 0 | | A1052 | 11.544 | 13.874 | 5.093 | 1.00 16.61 | 0 |
| ATOM | 400 | N | | | 10.006 | 12.383 | 4.394 | 1.00 15.83 | N |
| MOTA | 401 | CA | | A1053 | 9.985 | 11.645 | 5.662 | 1.00 15.97 | C |
| ATOM | 402 | CB | | A1053 | 8.974 | 10.516 | 5.587 | 1.00 15.80 | C |
| MOTA . | 403 | C | | A1053 | 11.362 | 11.091 | 6.038 | 1.00 15.64 1.00 15.53 | 0 |
| ATOM | 404 | 0 | | A1053 | 11.750 | | 7.208 5.054 | 1.00 13.33 | N |
| MOTA | 405 | N | | A1054 | 12.094 | 10.573 | 5.327 | 1.00 14.89 | c |
| ATOM | 406 | CA | | A1054 | 13.420 | | 5.789 | 1.00 14.83 | c |
| ATOM | 407 | | | A1054 | 14.431 15.243 | 11.073 10.820 | 6.689 | 1.00 14.15 | 0 |
| ATOM | 408 | 0 | | A1054 A1055 | 14.403 | | 5.169 | 1.00 14.68 | N |
| ATOM | 409 | N | | A1055 | 15.327 | | 5.553 | 1.00 15.29 | C |
| ATOM | 410 | CA CB | | A1055 | 15.257 | | 4.533 | 1.00 14.70 | С |
| MOTA | 411 412 | CG | | A1055 | 16.364 | | 3.438 | 1.00 16.14 | С |
| ATOM | 413 | | | A1055 | 16.452 | | 2.658 | 1.00 16.61 | С |
| ATOM ATOM | 413 | NE | | A1055 | 17.610 | | 1.745 | | N |
| MOTA | 415 | CZ | | A1055 | 17.966 | | 1.021 | | С |
| ATOM | 416 | | | A1055 | 17.265 | | 1.093 | | N |
| ATOM | 417 | | | A1055 | 19.028 | | 0.215 | | N |
| ATOM | 418 | | | G A1055 | 15.010 | | 6.980 | 1.00 15.61 | С |
| ATOM | 419 | | | 3 A1055 | 15.909 | | 7.755 | 1.00 15.05 | 0 |
| | | | | | | | | • | |

| ATOM | 420 | N | TRP | A1056 | 13.731 | 13.826 | 7.333 | 1.00 15.92 | N |
|--------------|------------|----------|-----|----------------|------------------|------------------|------------------|--------------------------|--------|
| ATOM | 421 | CA | TRP | A1056 | 13.324 | 14.252 | 8.676 | 1.00 17.44 | C |
| ATOM | 422 | CB | | A1056 | 11.791 | 14.409 | 8.706 | 1.00 20.42 | C |
| MOTA | 423 | CG | TRP | A1056 | 11.151 | 14.202 | 10.044 | 1.00 24.52 | C |
| MOTA | 424 | CD2 | TRP | A1056 | 10.650 | 15.212 | 10.921 | 1.00 26.47 | C |
| MOTA | 425 | CE2 | TRP | A1056 | 10.140 | 14,556 | 12.065 | 1.00 27.71 | . C |
| MOTA | 426 | CE3 | TRP | A1056 | 10.581 | 16.607 | 10.854 | 1.00 27.13 | C |
| MOTA | 427 | CD1 | TRP | A1056 | 10.931 | 13.005 | 10.673 | 1.00 25.93 | C |
| MOTA | 428 | | | A1056 | 10.325 | 13.211 | 11.885 | 1.00 27.77 | И |
| ATOM | 429 | | | A1056 | 9.567 | 15.250 | 13.133 | 1.00 28.62 | C |
| ATOM | 430 | | | A1056 | 10.012 | 17.297 | 11.915 | 1.00 28.11 | C |
| MOTA | 431 | CH2 | | A1056 | 9.512 | 16.617 | 13.041 | 1.00 29.24 | C |
| MOTA | 432 | С | | A1056 | 13.807 | 13.259 | 9.758 | 1.00 16.63 | 0 |
| ATOM | 433 | 0 | | A1056 | 14.339 | 13.661 | 10.813 | 1.00 14.62 | |
| ATOM | 434 | N | | A1057 | 13.645 | 11.965 | 9.477 | 1.00 15.34 | N C |
| ATOM | 435 | CA | | A1057 | 14.034 | 10.892 | 10.404 | 1.00 14.89 | C |
| ATOM | 436 | CB | | A1057 | 13.509 | 9.549 | 9.864 | 1.00 16.31 1.00 15.29 | 0 |
| MOTA | 437 | OG | | A1057 | 13.653 | 8.482 | 10.792 | 1.00 14.80 | C |
| ATOM | 438 | С | | A1057 | 15.558 | 10.833 | 10.624 11.748 | 1.00 13.11 | ő |
| ATOM | 439 | 0 | | A1057 | 16.033 | 10.618 | | 1.00 13.11 | N |
| ATOM | 440 | N | | A1058 | 16.326 | 11.043 | 9.560 9.670 | 1.00 13.00 | c |
| ATOM | 441 | CA | | A1058 | 17.784 | 11.015 11.077 | 8.283 | 1.00 14.39 | Č |
| ATOM | 442 | CB | | A1058 | 18.408 | 12.162 | 10.528 | 1.00 14.33 | c |
| ATOM | 443 | С | | A1058 | 18.326 19.253 | 11.972 | 11.326 | 1.00 12.67 | Õ |
| ATOM | 444 | 0 | | A1058 | 17.760 | 13.356 | 10.346 | 1.00 14.25 | N |
| ATOM | 445 | N Cr | | A1059 | 18.198 | 14.530 | 11.102 | 1.00 14.23 | Ĉ |
| MOTA | 446 | CA | | A1059 A1059 | 17.561 | 15.807 | 10.511 | 1.00 14.63 | Č |
| ATOM | 447 | CB | | A1059 | 18.030 | 16.077 | 9.061 | 1.00 15.21 | С |
| ATOM | 448 | CG CD | | A1059 | 17.605 | 17.445 | 8.497 | 1.00 14.78 | Ċ |
| ATOM | 449 450 | CE | | A1059 | 18.198 | 17.662 | 7.096 | 1.00 15.27 | С |
| ATOM | 451 | NZ | | A1059 | 17.780 | 18.955 | 6.460 | 1.00 14.73 | N |
| ATOM ATOM | 452 | C | | A1059 | 17.902 | 14.382 | 12.597 | 1.00 15.88 | С |
| ATOM | 453 | Ö | | A1059 | 18.726 | 14.755 | 13.441 | 1.00 15.17 | 0 |
| ATOM | 454 | N | | A1060 | 16.743 | 13.819 | 12.933 | 1.00 15.81 | N |
| ATOM | 455 | CA | | A1060 | 16.395 | 13.609 | 14.337 | 1.00 16.66 | C |
| ATOM | 456 | СВ | | A1060 | 14.943 | 13.142 | 14.474 | 1.00 18.92 | C |
| ATOM | 457 | CG | | A1060 | 13.922 | 14.183 | 14.023 | 1.00 23.44 | C |
| ATOM | 458 | CD | GLU | A1060 | 12.804 | 14.369 | 15.031 | 1.00 26.75 | С |
| ATOM | 459 | OE1 | GLU | A1060 | 12.175 | 13.358 | 15.414 | 1.00 29.16 | 0 |
| MOTA | 460 | OE2 | GLU | A1060 | 12.547 | 15.522 | 15.437 | 1.00 27.98 | 0 |
| MOTA | 461 | С | GLU | A1060 | 17.333 | 12.578 | 14.977 | 1.00 15.69 | С |
| ATOM | 462 | 0 | GLU | A1060 | 17.740 | 12.730 | 16.138 | 1.00 14.40 | 0 |
| ATOM | 463 | N | ALA | A1061 | 17.689 | | 14.219 | 1.00 14.51 | N |
| ATOM | 464 | CA | ALA | A1061 | 18.586 | 10.500 | 14.727 | 1.00 14.88 | C |
| MOTA | 465 | CB | ALA | A1061 | 18.658 | 9.312 | 13.730 | 1.00 14.28 | C |
| ATOM | 466 | С | | A1061 | 19.998 | 11.037 | 15.018 | 1.00 15.17 | C |
| MOTA | 467 | 0 | | A1061 | 20.635 | | 16.001 | 1.00 14.05 | 0 |
| MOTA | 468 | N | | E A1062 | 20.488 | | 14.167 | 1.00 14.78 | N C |
| MOTA | 469 | CA | | E A1062 | 21.811 | | 14.365 | 1.00 16.06 | C |
| MOTA | 470 | CB | | E A1062 | 22.200 | | 13.161 | 1.00 16.25 | |
| ATOM | 471 | CG | | E A1062 | 23.514 | | 13.341 | 1.00 17.02 | C |
| ATOM | 472 | | | E A1062 | 23.562 | | 14.039 | 1.00 17.84 1.00 16.96 | c |
| MOTA | 473 | | | E A1062 | 24.707 | | 12.847 | 1.00 16.96 | . c |
| MOTA | 474 | | | E A1062 | 24.783 | | 14.247 | | . c |
| MOTA | 475 | | | E A1062 | 25.931 | | 13.049 13.754 | | c |
| MOTA | 476 | CZ | PHI | E A1062 | 25.964 | 15.505 | 13.134 | 1.00 10.07 | · |

| A TOM | 477 | С | DUE | A1062 | 21.830 | 13.380 | 15.651 | 1.00 16.47 | | С |
|-------|-----|-----|-----|---------|--------|--------|--------|------------|---|-----|
| ATOM | | | | A1062 | 22.792 | 13.326 | 16.422 | 1.00 15.43 | | Ö |
| ATOM | 478 | | | | | 14.138 | 15.895 | 1.00 17.69 | | N |
| ATOM | 479 | | | A1063 | 20.760 | | | | | |
| ATOM | 480 | | | A1063 | 20.695 | 14.979 | 17.093 | 1.00 19.00 | | C |
| ATOM | 481 | СВ | | A1063 | 19.446 | 15.881 | 17.067 | 1.00 20.22 | | C |
| ATOM | 482 | OG | SER | A1063 | 18.276 | 15.162 | 17.434 | 1.00 23.89 | | 0 |
| ATOM | 483 | С | SER | A1063 | 20.707 | 14.148 | 18.383 | 1.00 19.17 | | С |
| ATOM | 484 | 0 | SER | A1063 | 21.229 | 14.602 | 19.405 | 1.00 19.65 | | 0 |
| ATOM | 485 | N | LYS | A1064 | 20.124 | 12.949 | 18.353 | 1.00 18.93 | | N |
| ATOM | 486 | CA | LYS | A1064 | 20.121 | 12.093 | 19.545 | 1.00 19.27 | | С |
| ATOM | 487 | | | A1064 | 19.094 | 10.961 | 19.418 | 1.00 19.83 | | С |
| ATOM | 488 | CG | | A1064 | 17.648 | 11.413 | 19.471 | 1.00 21.72 | | С |
| ATOM | 489 | CD | | A1064 | 16.720 | 10.201 | 19.456 | 1.00 23.02 | | С |
| | | | | A1064 | 15.270 | 10.614 | 19.240 | 1.00 24.30 | | С |
| ATOM | 490 | | | | 14.379 | 9.425 | 19.074 | 1.00 25.01 | | N |
| ATOM | 491 | NZ | | A1064 | | 11.497 | 19.770 | 1.00 23.01 | | C |
| ATOM | 492 | C | | A1064 | 21.510 | | | | | Ö |
| ATOM | 493 | 0 | | A1064 | 21.920 | 11.256 | 20.922 | 1.00 18.44 | | |
| ATOM | 494 | N | | A1065 | 22.230 | 11.254 | 18.674 | 1.00 18.91 | | N |
| MOTA | 495 | CA | | A1065 | 23.588 | 10.716 | 18.757 | 1.00 20.48 | | C |
| MOTA | 496 | CB | ALA | A1065 | 24.110 | 10.348 | 17.359 | 1.00 19.55 | | C |
| MOTA | 497 | С | ALA | A1065 | 24.515 | 11.745 | 19.417 | 1.00 22.05 | | С |
| MOTA | 498 | 0 | ALA | A1065 | 25.486 | 11.374 | 20.086 | 1.00 22.04 | | 0 |
| ATOM | 499 | N | MET | A1066 | 24.224 | 13.032 | 19.224 | 1.00 23.48 | | N |
| MOTA | 500 | CA | MET | A1066 | 25.027 | 14.101 | 19.836 | 1.00 26.32 | | С |
| ATOM | 501 | CB | | A1066 | 24.893 | 15.409 | 19.044 | 1.00 27.55 | | С |
| ATOM | 502 | CG | | A1066 | 25.471 | 15.377 | 17.634 | 1.00 29.85 | | С |
| ATOM | 503 | SD | | A1066 | 27.227 | 15.839 | 17.541 | 1.00 34.49 | | S |
| | 504 | CE | | A1066 | 27.100 | 17.585 | 17.194 | 1.00 32.80 | | С |
| ATOM | | | | | 24.554 | 14.334 | 21.277 | 1.00 27.22 | | č |
| ATOM | 505 | C | | A1066 | | 14.916 | 22.093 | 1.00 27.02 | | ŏ |
| MOTA | 506 | 0 | | A1066 | 25.272 | | | 1.00 27.02 | • | N |
| MOTA | 507 | N | | A1067 | 23.335 | 13.885 | 21.572 | | | C |
| ATOM | 508 | CA | | A1067 | 22.770 | 14.032 | 22.905 | 1.00 29.77 | | C |
| ATOM | 509 | С | | A1067 | 22.161 | 15.395 | 23.194 | 1.00 31.30 | | 0 |
| ATOM | 510 | 0 | | A1067 | 21.943 | 15.746 | 24.356 | 1.00 30.88 | | N |
| MOTA | 511 | N | | A1068 | 21.857 | 16.153 | 22.145 | 1.00 32.65 | | |
| MOTA | 512 | CA | | A1068 | 21.305 | 17.495 | 22.309 | 1.00 34.08 | | C |
| ATOM | 513 | CB | | A1068 | 22.128 | 18.520 | 21.510 | 1.00 34.54 | | C |
| ATOM | 514 | | | A1068 | 21.950 | 18.280 | 20.109 | 1.00 34.50 | | 0 |
| MOTA | 515 | CG2 | THR | A1068 | 23.613 | 18.400 | 21.849 | 1.00 34.68 | | C |
| ATOM | 516 | С | THR | A1068 | 19.843 | 17.694 | 21.911 | 1.00 35.08 | | C |
| MOTA | 517 | 0 | THR | A1068 | 19.199 | 18.637 | 22.380 | 1.00 35.34 | | 0 |
| ATOM | 518 | N | GLY | A1069 | 19.320 | 16.834 | 21.046 | 1.00 35.84 | | N |
| ATOM | 519 | CA | GLY | A1069 | 17.942 | 16.995 | 20.611 | 1.00 37.37 | | С |
| ATOM | 520 | С | GLY | A1069 | 17.855 | 18.092 | 19.561 | 1.00 38.51 | | С |
| ATOM | 521 | 0 | GLY | A1069 | 18.739 | 18.946 | 19.478 | 1.00 38.69 | | 0 |
| ATOM | 522 | N | | A1070 | 16.801 | 18.088 | 18.752 | 1.00 39.34 | | N |
| ATOM | 523 | CA | | A1070 | 16.688 | 19.108 | 17.722 | 1.00 40.39 | | C |
| ATOM | 524 | СВ | | A1070 | 16.453 | 18.482 | 16.329 | 1.00 40.56 | | С |
| ATOM | 525 | | | A1070 | 15.019 | 17.992 | 16.207 | 1.00 40.43 | | С |
| MOTA | 526 | | | A1070 | 16.784 | 19.515 | 15.245 | 1.00 40.90 | | . C |
| ATOM | 527 | | | A1070 | 16.900 | 18.947 | 13.841 | 1.00 40.92 | | С |
| | 528 | CDI | | A1070 | 15.616 | | 18.019 | 1.00 41.07 | | С |
| ATOM | | | | A1070 | 14.461 | 19.826 | 18.305 | 1.00 41.30 | | o |
| ATOM | 529 | 0 | | | 16.046 | | 17.936 | 1.00 41.96 | | N |
| ATOM | 530 | N | | R A1071 | | | 18.201 | 1.00 41.30 | | C |
| ATOM | 531 | CA | | R A1071 | 15.247 | | 19.271 | 1.00 42.87 | | c |
| ATOM | 532 | CB | | R A1071 | 14.184 | 22.325 | 20.496 | 1.00 43.28 | | Ö |
| ATOM | 533 | OG | SEF | R A1071 | 14.779 | 21.937 | 20.496 | 1.00 44.31 | | 0 |

| ATOM | 534 | С | SER | A1071 | 16.314 | 23.521 | 18.753 | 1.00 43.09 | С |
|------|-----|---------|------|---------|--------|--------|--------|------------|---|
| ATOM | 535 | | | A1071 | 16.254 | 24.741 | 18.585 | 1.00 43.47 | Ō |
| | | | | | | 22.914 | 19.419 | 1.00 42.86 | Ŋ |
| ATOM | 536 | | | A1072 | 17.295 | | 19.419 | 1.00 42.57 | C |
| ATOM | 537 | | | A1072 | 18.427 | 23.637 | | | C |
| MOTA | 538 | | | A1072 | 19.143 | 22.768 | 21.022 | 1.00 42.32 | |
| ATOM | 539 | | | A1072 | 18.214 | 22.218 | 22.093 | 0.05 42.40 | С |
| ATOM | 540 | | | A1072 | 17.501 | 23.339 | 22.829 | 0.05 42.37 | C |
| ATOM | 541 | CE | LYS | A1072 | 16.446 | 22.789 | 23.773 | 0.05 42.36 | С |
| ATOM | 542 | NZ | LYS | A1072 | 15.708 | 23.878 | 24.472 | 0.05 42.34 | N |
| ATOM | 543 | С | LYS | A1072 | 19.330 | 23.904 | 18.783 | 1.00 42.27 | С |
| ATOM | 544 | 0 | LYS. | A1072 | 20.222 | 24.752 | 18.814 | 1.00 42.17 | 0 |
| ATOM | 545 | N | LEU | A1073 | 19.065 | 23.149 | 17.723 | 1.00 41.69 | N |
| ATOM | 546 | CA | LEU | A1073 | 19.773 | 23.255 | 16.458 | 1.00 41.03 | С |
| ATOM | 547 | СВ | | A1073 | 20.879 | 22.197 | 16.365 | 1.00 41.27 | С |
| ATOM | 548 | CG | | A1073 | 21.578 | 22.058 | 15.008 | 1.00 41.68 | С |
| ATOM | 549 | | | A1073 | 23.024 | 21.623 | 15.193 | 1.00 41.49 | С |
| ATOM | 550 | | | A1073 | 20.819 | 21.060 | 14.156 | 1.00 41.59 | С |
| ATOM | 551 | C | | A1073 | 18.696 | 23.006 | 15.408 | 1.00 39.74 | C |
| | 552 | | | A1073 | 17.999 | 21.994 | 15.458 | 1.00 40.51 | Ō |
| ATOM | | 0 | | A1073 | 18.550 | 23.937 | 14.473 | 1.00 37.90 | N |
| ATOM | 553 | N C7 | | | 17.532 | 23.795 | 13.452 | 1.00 34.96 | Ċ |
| ATOM | 554 | CA | | A1074 | | | 12.399 | 1.00 34.30 | Č |
| ATOM | 555 | С | | A1074 | 17.853 | 22.756 | | | 0 |
| MOTA | 556 | 0 | | A1074 | 18.968 | 22.237 | 12.331 | 1.00 31.86 | |
| ATOM | 557 | N | | A1075 | 16.861 | 22.447 | 11.575 | 1.00 30.76 | N |
| ATOM | 558 | CA | | A1075 | 17.047 | 21.474 | 10.510 | 1.00 29.13 | C |
| ATOM | 559 | CB | | A1075 | 15.691 | 21.061 | 9.913 | 1.00 28.59 | C |
| ATOM | 560 | CG | | A1075 | 14.795 | 20.317 | 10.871 | 1.00 28.14 | C |
| ATOM | 561 | | | A1075 | 14.129 | 20.990 | 11.893 | 1.00 28.80 | C |
| MOTA | 562 | | | A1075 | 14.617 | 18.940 | 10.747 | 1.00 27.48 | C |
| ATOM | 563 | | | A1075 | 13.294 | 20.301 | 12.780 | 1.00 28.53 | C |
| ATOM | 564 | CE2 | PHE | A1075 | 13.787 | | 11.624 | 1.00 28.38 | С |
| ATOM | 565 | CZ | PHE | A1075 | 13.123 | 18.921 | 12.644 | 1.00 28.31 | C |
| MOTA | 566 | С | PHE | A1075 | 17.940 | 22.039 | 9.402 | 1.00 27.80 | C |
| ATOM | 567 | 0 | PHE | A1075 | 18.556 | 21.280 | 8.655 | 1.00 27.44 | 0 |
| ATOM | 568 | N | GLN | A1076 | 18.022 | 23.366 | 9.301 | 1.00 26.94 | N |
| ATOM | 569 | CA | GLN | A1076 | 18.828 | 24.003 | 8.250 | 1.00 26.57 | C |
| MOTA | 570 | CB | GLN | A1076 | 18.468 | 25.490 | 8.111 | 1.00 27.23 | С |
| ATOM | 571 | CG | GLN | A1076 | 17.037 | 25.783 | 7.655 | 1.00 28.06 | С |
| MOTA | 572 | CD | GLN | A1076 | 16.725 | 25.253 | 6.261 | 1.00 28.68 | С |
| MOTA | 573 | OE1 | GLN | A1076 | 17.504 | 25.432 | 5.321 | 1.00 28.59 | 0 |
| ATOM | 574 | NE2 | GLN | A1076 | 15.571 | 24.616 | 6.119 | 1.00 28.78 | N |
| ATOM | 575 | C | GLN | A1076 | 20.341 | 23.880 | 8.435 | 1.00 26.18 | С |
| ATOM | 576 | 0 | GLN | A1076 | 21.110 | 24.292 | 7.565 | 1.00 25.59 | 0 |
| MOTA | 577 | N | ASP | A1077 | 20.774 | 23.318 | 9.558 | 1.00 25.77 | N |
| ATOM | 578 | CA | ASP | A1077 | 22.204 | 23.158 | 9.808 | 1.00 25.68 | С |
| ATOM | 579 | CB | ASP | A1077 | 22.498 | 23.399 | 11.287 | 1.00 28.73 | С |
| ATOM | 580 | CG | ASP | A1077 | 23.952 | 23.697 | 11.542 | 1.00 30.84 | С |
| ATOM | 581 | OD1 | ASP | A1077 | 24.457 | 24.688 | 10.969 | 1.00 33.09 | 0 |
| ATOM | 582 | OD2 | ASF | A1077 | 24.590 | 22.947 | 12.309 | 1.00 32.53 | 0 |
| ATOM | 583 | С | ASF | A1077 | 22.729 | 21.770 | 9.393 | 1.00 24.42 | С |
| ATOM | 584 | 0 | ASE | A1077 | 23.928 | 21.487 | 9.516 | 1.00 23.80 | 0 |
| ATOM | 585 | N | LEU | A1078 | 21.831 | 20.919 | 8.899 | 1.00 22.23 | N |
| ATOM | 586 | CA | | A1078 | 22.187 | 19.559 | 8.463 | 1.00 20.68 | С |
| ATOM | 587 | CB | | A1078 | 21.530 | 18.525 | 9.398 | 1.00 19.99 | C |
| ATOM | 588 | CG | | J A1078 | 21.781 | 18.646 | 10.911 | 1.00 19.68 | С |
| ATOM | 589 | | | J A1078 | 20.853 | 17.703 | 11.686 | 1.00 19.87 | C |
| ATOM | 590 | | | J A1078 | 23.241 | 18.328 | 11.221 | 1.00 20.17 | C |
| | | | | | | | | | |

| ATOM | 591 | С | LEU | A1078 | 21.706 | 19.326 | 7.022 | 1.00 20.16 | С |
|---------|-------|------|-----|--------|--------|--------|--------|------------|----|
| ATOM | 592 | 0 | LEU | A1078 | 20.708 | 19.915 | 6.605 | 1.00 19.88 | 0 |
| ATOM | 593 | N | | A1079 | 22.408 | 18.474 | 6.265 | 1.00 19.89 | N |
| ATOM | 594 | CA | | A1079 | 22.021 | 18.165 | 4.875 | 1.00 18.83 | С |
| ATOM | 595 | СВ | | A1079 | 22.690 | 19.153 | 3.905 | 1.00 19.73 | С |
| ATOM | 596 | CG | | A1079 | 22.172 | 19.085 | 2.459 | 1.00 21.03 | Č |
| ATOM | 597 | CD | | A1079 | 22.914 | 20.028 | 1.510 | 1.00 22.47 | Ċ |
| ATOM | 598 | | | A1079 | 24.127 | 19.815 | 1.271 | 1.00 22.27 | 0 |
| ATOM | 599 | | | A1079 | 22.279 | 20.982 | 1.002 | 1.00 23.12 | o |
| | | | | | 22.385 | 16.716 | 4.484 | 1.00 23.12 | Č |
| ATOM | 600 | C | | A1079 | | | | 1.00 17.37 | 0 |
| ATOM | 601 | 0 | | A1079 | 23.492 | 16.242 | 4.778 | | |
| MOTA | 602 | N | | A1080 | 21.451 | 16.023 | 3.826 | 1.00 16.74 | N |
| MOTA | 603 | CA | | A1080 | 21.644 | 14.626 | 3.396 | 1.00 16.37 | C |
| MOTA | 604 | СВ | | A1080 | 20.633 | 13.675 | 4.138 | 1.00 16.24 | C |
| MOTA | 605 | | | A1080 | 20.859 | 12.217 | 3.738 | 1.00 16.31 | C |
| ATOM | 606 | | | A1080 | 20.776 | 13.832 | 5.654 | 1.00 16.73 | C |
| MOTA | 607 | С | | A1080 | 21.454 | 14.439 | 1.868 | 1.00 16.11 | С |
| ATOM | 608 | 0 | VAL | A1080 | 20.356 | 14.635 | 1.357 | 1.00 16.59 | 0 |
| ATOM | 609 | N | LEU | A1081 | 22.519 | 14.060 | 1.155 | 1.00 16.23 | N |
| MOTA | 610 | CA | LEU | A1081 | 22.473 | 13.830 | -0.303 | 1.00 16.11 | С |
| ATOM | 611 | CB | LEU | A1081 | 23.488 | 14.749 | -1.017 | 1.00 16.03 | C |
| ATOM | 612 | CG | LEU | A1081 | 23.400 | 16.265 | -0.767 | 1.00 17.13 | C |
| ATOM | 613 | CD1 | LEU | A1081 | 24.565 | 16.983 | -1.464 | 1.00 16.85 | С |
| ATOM | 614 | CD2 | LEU | A1081 | 22.064 | 16.798 | -1.283 | 1.00 17.61 | C |
| ATOM | 615 | С | | A1081 | 22.790 | 12.350 | -0.624 | 1.00 16.47 | С |
| ATOM | 616 | 0 | | A1081 | 22.881 | 11.530 | 0.285 | 1.00 15.85 | 0 |
| ATOM | 617 | N | | A1082 | 22.954 | 12.004 | | 1.00 17.23 | N |
| ATOM | 618 | CA | | A1082 | 23.266 | 10.615 | -2.299 | 1.00 18.16 | C |
| ATOM | 619 | CB | | A1082 | 22.169 | 10.064 | -3.227 | 1.00 19.47 | c |
| ATOM | 620 | CG | | A1082 | 20.853 | 9.800 | -2.496 | 1.00 20.37 | c |
| | 621 | | | A1082 | 20.701 | 8.793 | -1.806 | 1.00 23.12 | ő |
| MOTA | | | | A1082 | 19.908 | 10.709 | -2.637 | 1.00 23.12 | Ŋ |
| ATOM | 622 | | | | | 10.709 | | 1.00 21.10 | C |
| ATOM | 623 | C | | A1082 | 24.633 | | | | Ö |
| ATOM | 624 | 0 | | A1082 | 24.894 | 11.311 | -3.936 | 1.00 18.53 | |
| ATOM | 625 | N | | A1083 | 25.501 | 9.621 | -2.567 | 1.00 18.47 | N |
| ATOM | 626 | CA | | A1083 | 26.840 | 9.496 | -3.160 | 1.00 19.58 | C |
| ATOM | 627 | CB | | A1083 | 27.823 | 8.831 | -2.172 | 1.00 19.14 | C |
| ATOM | 628 | CG | | A1083 | 27.525 | 7.354 | -1.898 | 1.00 19.47 | C |
| ATOM | 629 | | | A1083 | 28.000 | 6.806 | -0.896 | 1.00 21.52 | 0 |
| MOTA | 630 | ND2 | | A1083 | 26.774 | 6.705 | -2.778 | 1.00 18.08 | N |
| ATOM | 631 | С | | A1083 | 26.879 | 8.801 | -4.522 | 1.00 21.02 | C |
| ATOM | 632 | 0 | | A1083 | 25.835 | 8.408 | -5.053 | 1.00 20.46 | 0 |
| ATOM | 633 | N | | A1084 | 28.073 | 8.655 | -5.095 | 1.00 22.56 | И |
| ATOM | 634 | CA | GLU | A1084 | 28.183 | 8.048 | -6.422 | 1.00 25.48 | С |
| ATOM | 635 | CB | GLU | A1084 | 29.606 | 8.243 | | 1.00 26.01 | С |
| MOTA | 636 | CG | | A1084 | 30.704 | 7.346 | -6.452 | 1.00 27.48 | С |
| ATOM | 637 | CD | GLU | A1084 | 32.055 | 7621 | -7.127 | 1.00 28.81 | С |
| ATOM | 638 | OE1 | GLU | A1084 | 32.087 | 7.807 | -8.365 | 1.00 28.44 | 0 |
| MOTA | 639 | OE2 | GLU | A1084 | 33.085 | 7.644 | -6.424 | 1.00 29.66 | 0 |
| ATOM | 640 | С | GLU | A1084 | 27.747 | 6.583 | -6.523 | 1.00 26.10 | С |
| ATOM | 641 | 0 | GLU | A1084 | 27.675 | 6.030 | -7.618 | 1.00 26.96 | 0 |
| ATOM | 642 | N | | A1085 | 27.446 | 5.958 | -5.390 | 1.00 26.87 | N |
| ATOM | 643 | CA | | A1085 | 26.976 | 4.571 | -5.381 | 1.00 27.01 | С |
| ATOM | 644 | CB | | A1085 | 27.697 | 3.761 | -4.302 | 1.00 29.89 | C |
| ATOM | 645 | CG | | A1085 | 29.210 | 3.670 | -4.479 | 1.00 33.27 | c |
| ATOM | 646 | CD | | A1085 | 29:603 | 2.687 | -5.570 | 1.00 35.91 | Ċ |
| ATOM | 647 | NE | | A1085 | 31.041 | 2.724 | -5.834 | 1.00 37.82 | N |
| 111 011 | O-7 ' | 1477 | | ****** | 21.041 | 2.127 | 3.034 | 1.00 57.02 | ., |

| ATOM | 648 | CZ | ARG | A1085 | 31.696 | 1.814 | -6.549 | 1.00 39.02 | С |
|------|-----|-----|-----|---------|------------------|--------|--------|------------|---|
| ATOM | 649 | NH1 | ARG | A1085 | 33.005 | 1.929 | -6.739 | 1.00 39.21 | N |
| ATOM | 650 | NH2 | ARG | A1085 | 31.043 | 0.782 | -7.067 | 1.00 39.98 | N |
| ATOM | 651 | С | ARG | A1085 | 25.467 | 4.573 | -5.097 | 1.00 26.06 | C |
| ATOM | 652 | 0 | ARG | A1085 | 24.830 | 3.515 | -5.033 | 1.00 26.15 | 0 |
| ATOM | 653 | N | GLY | A1086 | 24.911 | 5.768 | -4.907 | 1.00 24.38 | N |
| ATOM | 654 | CA | GLY | A1086 | 23.485 | 5.910 | -4.649 | 1.00 22.84 | C |
| ATOM | 655 | C | | A1086 | 22.989 | 5.874 | -3.207 | 1.00 21.70 | Č |
| ATOM | 656 | 0 | | A1086 | 21.780 | 5.910 | -2.980 | 1.00 21.52 | Õ |
| ATOM | 657 | N | | A1087 | 23.896 | 5.813 | -2.234 | 1.00 20.27 | N |
| ATOM | 658 | CA | | A1087 | 23.506 | 5.757 | -0.819 | 1.00 19.12 | C |
| ATOM | 659 | СВ | | A1087 | 24.452 | 4.825 | -0.065 | 1.00 19.31 | c |
| ATOM | 660 | C | | A1087 | 23.468 | 7.126 | -0.123 | 1.00 13.31 | C |
| ATOM | 661 | Ō | | A1087 | 24.293 | 8.001 | -0.400 | 1.00 17.46 | Õ |
| ATOM | 662 | N | | A1088 | 22.511 | 7.322 | 0.807 | 1.00 17.16 | Ŋ |
| ATOM | 663 | CD | | A1088 | 21.424 | 6.400 | 1.186 | 1.00 17.79 | C |
| ATOM | 664 | CA | | A1088 | 22.398 | 8.598 | 1.529 | 1.00 16.21 | C |
| ATOM | 665 | CB | | A1088 | 21.053 | 8.469 | 2.263 | 1.00 16.21 | C |
| ATOM | 666 | CG | | A1088 | 20.938 | 6.995 | 2.507 | 1.00 18.47 | |
| ATOM | 667 | C | | A1088 | 23.579 | 8.828 | 2.481 | 1.00 17.39 | C |
| ATOM | 668 | 0 | | A1088 | 24.084 | 7.876 | 3.082 | 1.00 13.33 | |
| ATOM | 669 | N | | A1089 | | 10.085 | | | 0 |
| ATOM | 670 | CA | | A1089 | 24.018 25.148 | | 2.597 | 1.00 14.68 | N |
| ATOM | 671 | | | | | 10.453 | 3.466 | 1.00 15.17 | C |
| ATOM | 672 | CB | | A1089 | 26.478 | 10.205 | 2.728 | 1.00 15.96 | C |
| ATOM | 673 | CG | | A1089 | 26.834 | 11.280 | 1.707 | 1.00 17.14 | C |
| | | | | A1089 | 27.815 | 12.240 | 1.980 | 1.00 17.14 | C |
| ATOM | 674 | | | A1089 | 28.136 | 13.243 | 1.042 | 1.00 17.71 | C |
| ATOM | 675 | | | A1089 | 26.180 | 11.345 | 0.476 | 1.00 17.70 | C |
| ATOM | 676 | | | A1089 | 26.490 | 12.342 | -0.470 | 1.00 18.23 | C |
| ATOM | 677 | CZ | | A1089 | 27.467 | 13.286 | -0.180 | 1.00 18.79 | C |
| ATOM | 678 | ОН | | A1089 | 27.769 | 14.272 | -1.110 | 1.00 18.83 | 0 |
| ATOM | 679 | C | | A1089 | 25.068 | 11.931 | 3.886 | 1.00 15.23 | С |
| ATOM | 680 | 0 | | A1089 | 24.480 | 12.749 | 3.172 | 1.00 14.55 | 0 |
| ATOM | 681 | N | | A1090 | 25.664 | 12.276 | 5.030 | 1.00 15.03 | N |
| ATOM | 682 | CA | | A1090 | 25.646 | 13.668 | 5.502 | 1.00 16.07 | С |
| ATOM | 683 | CB | | A1090 · | | 13.743 | 7.023 | 1.00 15.87 | C |
| ATOM | 684 | CG | | A1090 | 24.662 | 13.469 | 7.864 | 1.00 15.54 | C |
| ATOM | 685 | | | A1090 | 24.359 | 12.176 | 8.287 | 1.00 14.81 | С |
| ATOM | 686 | | | A1090 | 23.798 | 14.512 | 8.213 | 1.00 15.28 | C |
| MOTA | 687 | | | A1.090 | 23.207 | 11.920 | 9.048 | 1.00 15.40 | С |
| ATOM | 688 | | | A1090 | 22.643 | 14.272 | 8.973 | 1.00 16.17 | С |
| ATOM | 689 | CZ | | A1090 | 22.347 | 12.971 | 9.390 | 1.00 15.25 | С |
| ATOM | 690 | С | | A1090 | 26.694 | 14.553 | 4.800 | 1.00 16.94 | С |
| ATOM | 691 | 0 | | A1090 | 27.898 | 14.378 | 5.005 | 1.00 15.67 | 0 |
| ATOM | 692 | N | | A1091 | 26.233 | 15.499 | 3.983 | 1.00 18.05 | N |
| ATOM | 693 | CA | | A1091 | 27.135 | 16.421 | 3.285 | 1.00 20.04 | С |
| ATOM | 694 | .CB | | A1091 | 26.528 | 16.864 | 1.949 | 1.00 20.26 | С |
| ATOM | 695 | OG | | A1091 | 25.196 | 17.305 | 2.106 | 1.00 21.03 | 0 |
| ATOM | 696 | С | | A1091 | 27.456 | 17.653 | 4.143 | 1.00 20.79 | С |
| ATOM | 697 | 0 | | A1091 | 28.445 | 18.349 | 3.890 | 1.00 21.71 | 0 |
| ATOM | 698 | N | | A1092 | 26.606 | 17.930 | 5.133 | 1.00 20.94 | N |
| ATOM | 699 | CA | | A1092 | 26.810 | 19.049 | 6.062 | 1.00 21.39 | С |
| MOTA | 700 | CB | | A1092 | 25.958 | 20.265 | 5.665 | 1.00 23.27 | С |
| ATOM | 701 | CG | | A1092 | 26.267 | 20.898 | 4.305 | 1.00 25.76 | C |
| ATOM | 702 | CD | | A1092 | 27.623 | 21.589 | 4.244 | 1.00 27.71 | C |
| ATOM | 703 | | | A1092 | 28.044 | 22.248 | 5.197 | 1.00 29.37 | 0 |
| ATOM | 704 | NE2 | GLN | A1092 | 28.301 | 21.461 | 3.106 | 1.00 28.25 | N |

| MOTA | 705 | С | GLN | A1092 | 26.416 | 18.619 | 7.489 | 1.00 20.95 | С |
|------|-----|-----|-----|-------|--------|------------------|------------------|--------------------------|---|
| ATOM | 706 | 0 | GLN | A1092 | 25.340 | 18.064 | 7.689 | 1.00 20.12 | 0 |
| ATOM | 707 | N | ALA | A1093 | 27.290 | 18.868 | 8.466 | 1.00 20.33 | N |
| MOTA | 708 | CA | ALA | A1093 | 27.030 | 18.533 | 9.874 | 1.00 20.84 | С |
| ATOM | 709 | СВ | | A1093 | 26.874 | 17.013 | 10.046 | 1.00 20.16 | C |
| ATOM | 710 | С | | A1093 | 28.179 | 19.041 | 10.757 | 1.00 21.48 | Ċ |
| ATOM | 711 | 0 | | A1093 | 29.319 | 19.128 | 10.304 | 1.00 21.44 | ō |
| ATOM | 712 | N | | A1094 | 27.890 | 19.389 | 12.027 | 1.00 22.28 | Ŋ |
| ATOM | 713 | CD | | A1094 | 26.539 | 19.598 | 12.585 | 1.00 22.57 | c |
| ATOM | 714 | CA | | A1094 | 28.921 | 19.887 | 12.954 | 1.00 22.63 | Č |
| ATOM | 715 | CB | | A1094 | 28.125 | 20.803 | 13.876 | 1.00 22.88 | Č |
| ATOM | 716 | CG | | A1094 | 26.828 | 20.003 | 14.020 | 1.00 23.37 | C |
| ATOM | 717 | C | | A1094 | 29.678 | 18.791 | 13.731 | 1.00 23.05 | č |
| ATOM | 718 | Ö | | A1094 | 29.571 | 18.700 | 14.959 | 1.00 23.03 | 0 |
| ATOM | 719 | Ŋ | | A1095 | 30.446 | 17.976 | 13.009 | 1.00 22.89 | N |
| ATOM | 720 | CA | | A1095 | 31.232 | 16.883 | 13.590 | 1.00 22.89 | C |
| ATOM | 721 | CB | | A1095 | 30.341 | 15.639 | 13.767 | 1.00 22.67 | C |
| | 721 | | | | | | | | |
| ATOM | | CG | | A1095 | 31.067 | 14.436 | 14.307 | 1.00 22.55 | C |
| ATOM | 723 | | | A1095 | 31.374 | 13.360 14.385 | 13.474 | 1.00 22.34 1.00 22.13 | C |
| ATOM | 724 | | | A1095 | 31.462 | | 15.641 13.963 | | C |
| ATOM | 725 | | | A1095 | 32.068 | 12.250 | | 1.00 22.27 | C |
| ATOM | 726 | | | A1095 | 32.156 | 13.281 | 16.143 | 1.00 22.71 | C |
| ATOM | 727 | CZ | | A1095 | 32.461 | 12.209 | 15.300 | 1.00 22.51 | С |
| ATOM | 728 | C | | A1095 | 32.406 | 16.592 | 12.639 | 1.00 23.22 | C |
| ATOM | 729 | 0 | | A1095 | 32.221 | 16.574 | 11.426 | 1.00 23.38 | 0 |
| ATOM | 730 | N | | A1096 | 33.602 | 16.353 | 13.183 | 1.00 23.37 | N |
| ATOM | 731 | CA | | A1096 | 34.792 | 16.122 | 12.347 | 1.00 23.62 | C |
| ATOM | 732 | CB | | A1096 | 35.993 | 16.858 | 12.955 | 1.00 24.11 | С |
| ATOM | 733 | OG | | A1096 | 36.331 | 16.317 | 14.223 | 1.00 26.37 | 0 |
| ATOM | 734 | С | | A1096 | 35.233 | 14.691 | 12.000 | 1.00 23.23 | C |
| ATOM | 735 | 0 | | A1096 | 36.094 | 14.510 | 11.125 | 1.00 22.88 | 0 |
| ATOM | 736 | N | | A1097 | 34.670 | 13.686 | 12.669 | 1.00 22.73 | N |
| ATOM | 737 | CA | | A1097 | 35.043 | 12.304 | 12.391 | 1.00 21.96 | С |
| MOTA | 738 | С | | A1097 | 34.138 | 11.589 | 11.393 | 1.00 21.41 | c |
| ATOM | 739 | 0 | | A1097 | 33.518 | 12.232 | 10.555 | 1.00 21.73 | 0 |
| ATOM | 740 | N | | A1098 | 34.066 | 10.259 | 11.479 | 1.00 20.96 | N |
| ATOM | 741 | CA | | A1098 | 33.228 | 9.456 | 10.578 | 1.00 20.77 | C |
| ATOM | 742 | CB | | A1098 | 33.822 | 8.052 | 10.409 | 1.00 22.35 | C |
| ATOM | 743 | CG | | A1098 | 35.205 | 8.017 | 9.774 | 1.00 25.18 | C |
| MOTA | 744 | CD | | A1098 | 35.630 | 6.587 | 9.449 | 1.00 26.26 | C |
| ATOM | 745 | CE | | A1098 | 36.996 | 6.553 | 8.772 | 1.00 28.39 | С |
| MOTA | 746 | ΝZ | | A1098 | 37.332 | 5.194 | 8.258 | 1.00 28.94 | N |
| ATOM | 747 | C | | A1098 | 31.770 | 9.313 | 11.046 | 1.00 19.74 | C |
| ATOM | 748 | 0 | | A1098 | 31.517 | 9.064 | 12.224 | 1.00 19.90 | 0 |
| ATOM | 749 | N | | A1099 | 30.826 | 9.461 | 10.113 | 1.00 18.27 | N |
| ATOM | 750 | CA | | A1099 | 29.393 | 9.340 | 10.400 | 1.00 17.38 | C |
| ATOM | 751 | CB | | A1099 | 28.622 | 10.638 | 9.997 | 1.00 17.39 | C |
| ATOM | 752 | | | A1099 | 27.124 | 10.465 | 10.284 | 1.00 16.62 | C |
| MOTA | 753 | | | A1099 | 29.171 | 11.849 | 10.761 | 1.00 15.42 | C |
| MOTA | 754 | | | A1099 | 28.790 | 13.196 | 10.165 | 1.00 15.80 | С |
| MOTA | 755 | C | | A1099 | 28.777 | 8.164 | 9.607 | 1.00 17.23 | C |
| MOTA | 756 | 0 | | A1099 | 28.697 | 8.226 | 8.381 | 1.00 18.55 | 0 |
| ATOM | 757 | N | | A1100 | 28.356 | | 10.298 | 1.00 16.06 | N |
| ATOM | 758 | CA | | A1100 | 27.733 | | 9.641 | 1.00 15.73 | С |
| ATOM | 759 | CB | | A1100 | 28.163 | | 10.347 | 1.00 15.81 | С |
| ATOM | 760 | CG | | A1100 | 29.665 | 4.374 | 10.328 | 1.00 16.55 | C |
| ATOM | 761 | CD2 | TRP | A1100 | 30.415 | 3.750 | 9.274 | 1.00 16.48 | С |

| ATOM | 762 | CE2 | TRP | A1100 | 31.774 | 3.736 | 9.676 | 1.00 17.61 | С |
|--------------|------------|---------|-----|----------------|------------------|----------------|----------------|--------------------------|--------|
| ATOM | 763 | CE3 | TRP | A1100 | 30.071 | 3.199 | 8.030 | 1.00 17.03 | Ċ |
| ATOM | 764 | CD1 | TRP | A1100 | 30.575 | 4.704 | 11.300 | 1.00 17.00 | С |
| MOTA | 765 | NE1 | TRP | A1100 | 31.844 | 4.322 | 10.916 | 1.00 16.91 | · N |
| MOTA | 766 | CZ2 | TRP | A1100 | 32.792 | 3.191 | 8.873 | 1.00 17.99 | С |
| MOTA | 767 | CZ3 | TRP | A1100 | 31.083 | 2.654 | 7.230 | 1.00 18.05 | С |
| MOTA | 768 | CH2 | TRP | A1100 | 32.430 | 2.656 | 7.659 | 1.00 17.40 | С |
| ATOM | 769 | С | TRP | A1100 | 26.190 | 6.079 | 9.705 | 1.00 15.39 | С |
| ATOM | 770 | 0 | TRP | A1100 | 25.638 | 6.160 | 10.801 | 1.00 15.11 | 0 |
| ATOM | 771 | N | LEU | A1101 | 25.517 | 6.100 | 8.545 | 1.00 14.54 | N |
| MOTA | 772 | CA | LEU | A1101 | 24.045 | 6.260 | 8.448 | 1.00 14.10 | С |
| MOTA | 773 | CB | LEU | A1101 | 23.705 | 7.658 | 7.883 | 1.00 14.83 | С |
| ATOM | 774 | CG | | A1101 | 22.267 | 7.893 | 7.366 | 1.00 15.12 | . С |
| ATOM | 775 | CD1 | LEU | A1101 | 21.330 | 8.116 | 8.541 | 1.00 15.77 | С |
| ATOM | 77,6 | | | A1101 | 22.216 | 9.105 | 6.427 | 1.00 15.58 | C |
| ATOM | 777 | С | | A1101 | 23.318 | 5.214 | 7.576 | 1.00 13.98 | С |
| ATOM | 778 | 0 | | A1101 | 23.847 | 4.789 | 6.537 | 1.00 13.24 | . 0 |
| ATOM | 779 | N | | A1102 | 22.109 | 4.808 | 7.996 | 1.00 13.49 | N |
| ATOM | 780 | CA | | A1102 | 21.278 | 3.857 | 7.226 | 1.00 14.16 | С |
| ATOM | 781 | CB | | A1102 | 21.525 | 2.411 | 7.683 | 1.00 14.32 | С |
| MOTA | 782 | OG | | A1102 | 20.947 | 1.471 | 6.781 | 1.00 14.30 | 0 |
| MOTA | 783 | С | | A1102 | 19.777 | 4.190 | 7.363 | 1.00 14.45 | С |
| ATOM | 784 | 0 | - | A1102 | 19.311 | 4.519 | 8.464 | 1.00 13.54 | 0 |
| ATOM | 785 | N | | A1103 | 19.029 | 4.089 | 6.254 | 1.00 14.69 | , И |
| MOTA | 786 | CA | | A1103 | 17.575 | 4.387 | 6.231 | 1.00 15.31 | C |
| ATOM | 787 | CB | | A1103 | 17.282 | 5.709 | 5.454 | 1.00 15.58 | C |
| ATOM | 788 | | | A1103 | 15.783 | 6.027 | 5.508 | 1.00 15.76 | C |
| MOTA | 789 | | | A1103 | 18.085 | 6.875 | 6.041 | 1.00 15.76 | С |
| ATOM | 790 | | | A1103 | 17.838 | 8.216 | 5.317 | 1.00 17.30 | C |
| ATOM | 791 792 | С | | A1103 | 16.766 | | 5.541 | 1.00 15.22 | C 0 |
| ATOM | 793 | 0 | | A1103 | 17.249 | 2.668 2.977 | 4.575 | 1.00 16.46 | И |
| ATOM ATOM | 794 | N CA | | A1104 A1104 | 15.550 14.686 | 1.926 | 6.023 5.429 | 1.00 15.94 1.00 17.08 | C |
| ATOM | 795 | CB | | | | 0.564 | 6.085 | 1.00 17.08 | C |
| ATOM | 796 | OG | | A1104 | 14.993 | -0.486 | 5.476 | 1.00 17.07 | 0 |
| ATOM | 797 | C | | A1104 | 13.174 | 2.248 | 5.574 | 1.00 17.16 | C |
| ATOM | 798 | 0 | | A1104 | 12.784 | 2.982 | 6.483 | 1.00 17.40 | 0 |
| ATOM | 799 | N | | A1104 | 12.704 | 1.699 | 4.698 | 1.00 18.34 | Ŋ |
| ATOM | 800 | CA | | A1105 | 10.877 | 1.989 | 4.776 | 1.00 19.13 | c |
| ATOM | 801 | CB | | A1105 | 10.572 | 3.300 | 4.041 | 1.00 20.61 | Ċ |
| ATOM | 802 | CG | | A1105 | 10.702 | 3.188 | 2.551 | 1.00 21.51 | č |
| ATOM | 803 | | | A1105 | 9.799 | 2.840 | 1.601 | 1.00 22.68 | Ċ |
| ATOM | 804 | | | A1105 | 11.906 | 3.333 | 1.896 | 1.00 23.14 | N |
| MOTA | 805 | | | A1105 | 11.742 | 3.075 | 0.610 | 1.00 23.36 | С |
| ATOM | 806 | | | A1105 | 10.473 | | | | N |
| ATOM | 807 | C | | A1105 | 9.918 | | 4.192 | 1.00 19.69 | С |
| ATOM | 808 | 0 | HIS | A1105 | 10.324 | 0.073 | 3.405 | 1.00 19.77 | 0 |
| ATOM | 809 | N | | A1106 | 8.640 | 1.034 | 4.577 | 1.00 20.07 | N |
| ATOM | 810 | CA | THR | A1106 | 7.564 | 0.171 | 4.056 | 1.00 20.65 | С |
| ATOM | 811 | CB | THR | A1106 | 6.941 | -0.769 | 5.131 | 1.00 20.02 | С |
| ATOM | 812 | OG1 | THR | A1106 | 6.198 | 0.004 | 6.085 | 1.00 19.30 | 0 |
| MOTA | 813 | CG2 | THR | A1106 | 8.029 | -1.578 | 5.852 | 1.00 19.90 | С |
| MOTA | 814 | С | THR | A1106 | 6.470 | 1.143 | 3.587 | 1.00 22.48 | С |
| ATOM | 815 | 0 | | A1106 | 6.720 | 2.347 | 3.476 | 1.00 21.87 | 0 |
| MOTA | 816 | N | | A1107 | 5.262 | 0.652 | 3.315 | 1.00 23.59 | N |
| ATOM | 817 | CA | | A1107 | 4.214 | 1.569 | 2.875 | 1.00 25.20 | С |
| MOTA | 818 | CB | ASP | A1107 | 3.146 | 0.831 | 2.052 | 1.00 27.87 | С |

| 3 mos. | ~ | ~~ | | | | | | | _ |
|--------|-----|------|-----|-------|----------|--------|--------|------------|---|
| ATOM | 819 | CG | | A1107 | 2.302 | -0.116 | 2.886 | 1.00 29.94 | С |
| ATOM | 820 | OD1 | ASP | A1107 | 1.331 | -0.672 | 2.332 | 1.00 32.47 | 0 |
| MOTA | 821 | OD2 | ASP | A1107 | 2.601 | -0.314 | 4.086 | 1.00 32.30 | 0 |
| ATOM | 822 | С | ASP | A1107 | 3.549 | 2.322 | 4.027 | 1.00 25.08 | С |
| ATOM | 823 | 0 | ASP | A1107 | 2.673 | 3.156 | 3.791 | 1.00 25.52 | 0 |
| ATOM | 824 | N | | A1108 | 3.965 | 2.042 | 5.264 | 1.00 24.18 | Ŋ |
| ATOM | 825 | CA | | A1108 | 3.380 | 2.703 | 6.435 | 1.00 23.78 | C |
| ATOM | 826 | | | | | | | 1.00 25.78 | |
| | | CB | | A1108 | 2.533 | 1.715 | 7.251 | | C |
| ATOM | 827 | CG | | A1108 | 1.283 | 1.211 | 6.550 | 1.00 28.60 | C |
| ATOM | 828 | CD | | A1108 | 0.375 | 0.426 | 7.479 | 1.00 30.45 | С |
| ATOM | 829 | | | A1108 | 0.768 | -0.606 | 8.026 | 1.00 31.65 | 0 |
| MOTA | 830 | NE2 | GLN | A1108 | -0.847 | 0.918 | 7.670 | 1.00 31.23 | N |
| MOTA | 831 | С | GLN | A1108 | 4.361 | 3.391 | 7.390 | 1.00 22.77 | С |
| ATOM | 832 | 0 | GLN | A1108 | 3.966 | 4.334 | 8.081 | 1.00 22.34 | 0 |
| ATOM | 833 | N | PHE | A1109 | 5.616 | 2.926 | 7.441 | 1.00 21.34 | N |
| MOTA | 834 | CA | PHE | A1109 | 6.633 | 3.513 | 8.342 | 1.00 20.67 | С |
| ATOM | 835 | СВ | | A1109 | 6.888 | 2.605 | 9.567 | 1.00 21.50 | Ċ |
| ATOM | 836 | CG | | A1109 | 5.654 | 2.213 | 10.328 | 1.00 22.53 | C |
| ATOM | 837 | | | A1109 | 4.947 | 1.059 | 9.989 | 1.00 23.72 | Č |
| | | | | | | | | | |
| ATOM | 838 | | | A1109 | 5.212 | 2.978 | 11.403 | 1.00 23.05 | С |
| ATOM | 839 | | | A1109 | 3.816 | 0.673 | 10.715 | 1.00 24.14 | C |
| ATOM | 840 | | | A1109 | 4.082 | 2.601 | 12.135 | 1.00 24.05 | C |
| ATOM | 841 | CZ | | A1109 | 3.383 | 1.445 | 11.789 | 1.00 23.64 | С |
| ATOM | 842 | С | | A1109 | 8.015 | 3.755 | 7.705 | 1.00 19.29 | С |
| ATOM | 843 | 0 | PHE | A1109 | 8.333 | 3.199 | 6.654 | 1.00 19.32 | 0 |
| ATOM | 844 | N | VAL | A1110 | 8.830 | 4.582 | 8.368 | 1.00 18.27 | N |
| MOTA | 845 | CA | VAL | A1110 | 10.218 | 4.864 | 7.955 | 1.00 16.90 | С |
| ATOM | 846 | CB | VAL | A1110 | 10.368 | 6.279 | 7.299 | 1.00 17.79 | С |
| ATOM | 847 | CG1 | VAL | A1110 | 10.126 | 7.377 | 8.325 | 1.00 17.09 | C |
| ATOM | 848 | | | A1110 | 11.754 | 6.428 | 6.681 | 1.00 17.98 | C |
| ATOM | 849 | С | | A1110 | 11.100 | 4.796 | 9.224 | 1.00 16.47 | Ċ |
| ATOM | 850 | Ö | | A1110 | 10.655 | 5.214 | 10.300 | 1.00 15.21 | ő |
| ATOM | 851 | N | | A1111 | 12.323 | 4.260 | 9.097 | 1.00 15.21 | N |
| ATOM | 852 | | | | 13.271 | 4.126 | 10.225 | | C |
| | | CA | | A1111 | | | | 1.00 16.10 | |
| ATOM | 853 | CB | | A1111 | 13.369 | 2.646 | 10.736 | 1.00 16.89 | C |
| MOTA | 854 | | | A1111 | 13.775 | 1.775 | 9.667 | 1.00 18.14 | 0 |
| ATOM | 855 | | | A1111 | 12.038 | 2.180 | | 1.00 18.11 | C |
| ATOM | 856 | С | | A1111 | 14.692 | 4.582 | 9.860 | 1.00 15.27 | С |
| MOTA | 857 | 0 | THR | A1111 | 15.082 | 4.502 | 8.690 | 1.00 14.78 | 0 |
| ATOM | 858 | N | ALA | A1112 | 15.462 | 5.041 | 10.858 | 1.00 14.23 | N |
| ATOM | 859 | CA · | ALA | A1112 | 16.845 | 5.505 | 10.639 | 1.00 13.59 | C |
| ATOM | 860 | CB | ALA | A1112 | 16.855 | 7.001 | 10.293 | 1.00 12.71 | С |
| ATOM | 861 | c ' | ALA | A1112 | 17.764 | 5.255. | 11.843 | 1.00 12.99 | С |
| ATOM | 862 | 0 | ALA | A1112 | 17.310 | 5.303 | 12.993 | 1.00 12.81 | 0 |
| ATOM | 863 | N | | A1113 | 19.055 | 5.032 | 11.570 | 1.00 12.47 | N |
| ATOM | 864 | CA | | A1113 | 20.064 | 4.761 | 12.610 | 1.00 13.04 | С |
| ATOM | 865 | СВ | | A1113 | 20.256 | 3.238 | 12.736 | 1.00 13.53 | c |
| ATOM | 866 | OG | | A1113 | 21.244 | 2.893 | 13.698 | 1.00 13.09 | Ō |
| ATOM | 867 | C | | A1113 | 21.427 | 5.444 | 12.318 | 1.00 13.78 | č |
| | | | | | | | | | |
| ATOM | 868 | 0 | | A1113 | 21.901 | 5.419 | 11.180 | 1.00 13.46 | 0 |
| ATOM | 869 | N | | A1114 | 22.048 | 6.039 | 13.348 | 1.00 13.44 | И |
| ATOM | 870 | CA | | A1114 | 23.349 | 6.735 | 13.208 | 1.00 12.85 | C |
| ATOM | 871 | CB | | A1114 | 23.151 | 8.288 | 13.286 | 1.00 12.88 | C |
| MOTA | 872 | | | A1114 | 24.496 | 9.005 | 13.384 | 1.00 12.82 | C |
| MOTA | 873 | CG2 | | A1114 | 22.384 | 8.794 | 12.056 | 1.00 13.36 | С |
| MOTA | 874 | С | | A1114 | . 24.393 | 6.328 | 14.278 | 1.00 12.70 | С |
| MOTA | 875 | 0 | VAL | A1114 | 24.045 | 6.140 | 15.444 | 1.00 12.48 | 0 |

| | 076 | | | | 05 660 | c 100 | 12 072 | 1 00 10 61 | |
|------|-----------------|-----|-----|-------|--------|--------|--------|------------|---|
| ATOM | 876 | N | | A1115 | 25.662 | 6.183 | 13.873 | 1.00 13.61 | N |
| ATOM | 877 | CA | ILE | A1115 | 26.765 | 5.846 | 14.800 | 1.00 13.97 | С |
| ATOM | 878 | CB | ILE | A1115 | 27.291 | 4.399 | 14.621 | 1.00 14.70 | С |
| ATOM | 87 9 | CG2 | ILE | A1115 | 28.393 | 4.124 | 15.653 | 1.00 15.55 | С |
| ATOM | 880 | CG1 | ILE | A1115 | 26.163 | 3.377 | 14.800 | 1.00 14.56 | C |
| ATOM | 881 | | | A1115 | 26.580 | 1.948 | 14.433 | 1.00 14.04 | С |
| ATOM | 882 | C | | A1115 | 27.940 | 6.786 | 14.502 | 1.00 15.39 | Ċ |
| ATOM | 883 | Ö | | A1115 | 28.372 | 6.879 | 13.348 | 1.00 14.30 | Ö |
| | | | | | | | | | |
| ATOM | 884 | N | | A1116 | 28.456 | 7.465 | 15.537 | 1.00 15.93 | N |
| ATOM | 885 | CA | | A1116 | 29.574 | 8.412 | 15.397 | 1.00 16.40 | C |
| ATOM | 886 | CB | | A1116 | 29.300 | 9.680 | 16.235 | 1.00 16.45 | С |
| ATOM | 887 | CG | | A1116 | 27.972 | 10.439 | 16.051 | 1.00 15.86 | С |
| ATOM | 888 | CD1 | LEU | A1116 | 27.935 | 11.642 | 16.994 | 1.00 16.47 | C |
| ATOM | 889 | CD2 | LEU | A1116 | 27.816 | 10.888 | 14.601 | 1.00 16.74 | C |
| ATOM | 890 | С | LEU | A1116 | 30.906 | 7.778 | 15.839 | 1.00 17.18 | С |
| ATOM | 891 | 0 | | A1116 | 30.973 | 7.125 | 16.880 | 1.00 15.82 | 0 |
| ATOM | 892 | N | | A1117 | 31.970 | 8.002 | 15.064 | 1.00 18.58 | N |
| ATOM | 893 | CA | | A1117 | 33.278 | 7.414 | 15.362 | 1.00 21.21 | C |
| ATOM | 894 | CB | | A1117 | 33.404 | 6.068 | 14.615 | 1.00 21.29 | Ċ |
| | | | | | | | | | C |
| ATOM | 895 | CG | | A1117 | 34.793 | 5.403 | 14.659 | 1.00 21.49 | |
| MOTA | 896 | CD | | A1117 | 34.930 | 4.238 | 13.675 | 1.00 21.22 | C |
| ATOM | 897 | OE1 | GLU | A1117 | 34.538 | 4.390 | 12.500 | 1.00 20.57 | 0 |
| MOTA | 898 | OE2 | GLU | A1117 | 35.446 | 3.166 | 14.064 | 1.00 22.68 | 0 |
| ATOM | 899 | С | GLU | A1117 | 34.487 | 8.290 | 15.001 | 1.00 23.59 | С |
| ATOM | 900 | 0 | GLU | A1117 | 34.440 | 9.108 | 14.083 | 1.00 22.02 | 0 |
| ATOM | 901 | N | GLU | A1118 | 35.576 | 8.115 | 15.740 | 1.00 27.34 | N |
| ATOM | 902 | CA | | A1118 | 36.801 | 8.839 | 15.429 | 1.00 31.25 | С |
| ATOM | 903 | CB | | A1118 | 36.859 | 10.184 | 16.157 | 1.00 33.00 | Ċ |
| ATOM | 904 | CG | | A1118 | 36.747 | 10.131 | 17.651 | 1.00 35.45 | Ċ |
| | | | | | | | 18.269 | 1.00 33.43 | č |
| ATOM | 905 | CD | | A1118 | 37.042 | 11.480 | | | |
| ATOM | 906 | OE1 | | A1118 | 36.389 | 12.470 | 17.874 | 1.00 38.60 | 0 |
| ATOM | 907 | | | A1118 | 37.932 | 11.551 | 19.145 | 1.00 39.01 | 0 |
| ATOM | 908 | С | GLU | A1118 | 38.005 | 7.964 | 15.764 | 1.00 33.04 | С |
| ATOM | 909 | 0 | GLU | A1118 | 38.074 | 7.358 | 16.835 | 1.00 33.37 | 0 |
| ATOM | 910 | N | ASN | A1119 | 38.928 | 7.875 | 14.809 | 1.00 34.80 | N |
| MOTA | 911 | CA | ASN | A1119 | 40.132 | 7.063 | 14.945 | 1.00 36.61 | С |
| ATOM | 912 | СВ | ASN | A1119 | 40.203 | 6.015 | 13.823 | 1.00 37.32 | C |
| ATOM | 913 | CG | ASN | A1119 | 38.862 | 5.356 | 13.537 | 1.00 38.38 | С |
| ATOM | 914 | OĐ1 | ASN | A1119 | 38.258 | 4.731 | 14.409 | 1.00 39.30 | 0 |
| ATOM | 915 | | | A1119 | 38.393 | 5.492 | 12.302 | 1.00 38.79 | N |
| ATOM | 916 | С | | A1119 | 41.354 | 7.972 | 14.845 | 1.00 37.29 | C |
| ATOM | 917 | Õ | | A1119 | 42.132 | 7.795 | 13.885 | 1.00 37.98 | 0 |
| ATOM | 918 | | | A1119 | 41.513 | 8.857 | 15.710 | 1.00 38.37 | ō |
| | | OAI | | | 41.313 | 0.037 | 13.710 | 1.00 30.37 | O |
| TER | 919 | | | A1119 | 27 510 | 2 057 | 21.175 | 1 00 00 67 | ~ |
| ATOM | 920 | CB | | B2003 | 37.510 | -3.957 | 21:175 | 1.00 28.67 | C |
| ATOM | 921 | CG | | B2003 | 37.230 | -5.443 | 21.092 | 1.00 31.61 | C |
| MOTA | 922 | SD | MET | B2003 | 38.381 | -6.420 | 22.089 | 1.00 36.00 | S |
| MOTA | 923 | CE | MET | B2003 | 37.478 | -6.538 | 23.632 | 1.00 34.64 | С |
| MOTA | 924 | С | MET | B2003 | 35.111 | -3.318 | 20.851 | 1.00 24.52 | С |
| MOTA | 925 | 0 | MET | B2003 | 34.821 | -3.223 | 22.044 | 1.00 23.78 | 0 |
| ATOM | 926 | N | MET | B2003 | 36.911 | -1.645 | 20.536 | 1.00 26.75 | N |
| ATOM | 927 | CA | | B2003 | 36.543 | -3.080 | 20.373 | 1.00 26.43 | C |
| ATOM | 928 | N | | B2004 | 34.220 | -3.611 | 19.907 | 1.00 23.33 | N |
| ATOM | 929 | CA | | B2004 | 32.814 | -3.877 | 20.214 | 1.00 21.77 | C |
| ATOM | 930 | CB | | B2004 | 31.948 | -3.818 | 18.923 | 1.00 22.25 | Č |
| | | | | B2004 | 30.528 | -4.317 | 19.214 | 1.00 21.40 | Č |
| ATOM | 931 | | | | | | | | c |
| MOTA | 932 | CGI | 114 | B2004 | 31.936 | -2.387 | 18.370 | 1.00 22.04 | C |

| MOTA | 933 | CD1 | ILE | B2004 | 31.248 | -2.242 | 17.013 | 1.00 23.31 | С |
|------|-----|-----|-----|-------|--------|--------|------------------|--------------------------|--------|
| MOTA | 934 | С | ILE | B2004 | 32.688 | -5.268 | 20.837 | 1.00 21.10 | С |
| MOTA | 935 | 0 | ILE | B2004 | 33.423 | -6.190 | 20.463 | 1.00 21.53 | 0 |
| ATOM | 936 | N | VAL | B2005 | 31.774 | -5.423 | 21.793 | 1.00 19.59 | , И |
| ATOM | 937 | CA | VAL | B2005 | 31.577 | -6.725 | 22.423 | 1.00 18.29 | С |
| ATOM | 938 | CB | VAL | B2005 | 32.240 | -6.783 | 23.834 | 1.00 18.82 | C |
| ATOM | 939 | CG1 | VAL | B2005 | 33.741 | -6.518 | 23.712 | 1.00 18.55 | С |
| ATOM | 940 | CG2 | VAL | B2005 | 31.596 | -5.776 | 24.778 | 1.00 19.42 | C |
| ATOM | 941 | С | VAL | B2005 | 30.108 | -7.189 | 22.520 | 1.00 17.17 | С |
| MOTA | 942 | 0 | VAL | B2005 | 29.827 | -8.180 | 23.193 | 1.00 16.88 | 0 |
| ATOM | 943 | N | | B2006 | 29.190 | -6.493 | 21.838 | 1.00 15.24 | N |
| ATOM | 944 | CA | | B2006 | 27.776 | -6.881 | 21.849 | 1.00 14.41 | С |
| ATOM | 945 | С | | B2006 | 26.800 | -5.899 | 21.191 | 1.00 13.76 | С |
| ATOM | 946 | ō | | B2006 | 27.067 | -4.703 | 21,177 | 1.00 12.82 | 0 |
| ATOM | 947 | N | | B2007 | 25.667 | -6.388 | 20.664 | 1.00 13.79 | N |
| ATOM | 948 | CA | | B2007 | 24.656 | -5.521 | 20.015 | 1.00 13.97 | С |
| ATOM | 949 | CB | | B2007 | 25.046 | -5.296 | 18.534 | 1.00 13.17 | С |
| ATOM | 950 | CG | | B2007 | 24.110 | -4.400 | 17.767 | 1.00 13.29 | С |
| ATOM | 951 | | | B2007 | 23.648 | -4.481 | 16.494 | 1.00 13.60 | С |
| MOTA | 952 | | | B2007 | 23.602 | -3.224 | 18.281 | 1.00 14.70 | N |
| MOTA | 953 | | | B2007 | 22.871 | -2.619 | 17.357 | 1.00 15.43 | C |
| ATOM | 954 | | | B2007 | 22.884 | | 16.262 | 1.00 13.92 | N |
| ATOM | 955 | C | | B2007 | 23.227 | -6.108 | 20.104 | 1.00 13.36 | Ċ |
| | | | | B2007 | 23.024 | -7.293 | 19.817 | 1.00 13.30 | ō |
| ATOM | 956 | 0 | | B2007 | 22.249 | -5.286 | 20.504 | 1.00 13.56 | N |
| ATOM | 957 | N | | | | -5.758 | 20.603 | 1.00 13.30 | c |
| ATOM | 958 | CA | | B2008 | 20.870 | | 20.407 | 1.00 13.42 | c |
| ATOM | 959 | C | | B2008 | 19.760 | -4.724 | | 1.00 13.33 | 0 |
| ATOM | 960 | 0 | | B2008 | 19.921 | -3.566 | 20.786 | | N |
| ATOM | 961 | N | | B2009 | 18.630 | -5.143 | 19.827 19.601 | 1.00 13.48 1.00 13.81 | C |
| ATOM | 962 | CA | | B2009 | 17.476 | -4.253 | 18.086 | 1.00 13.81 | č |
| ATOM | 963 | CB | | B2009 | 17.327 | -3.864 | | 1.00 14.27 | C |
| ATOM | 964 | | | B2009 | 18.651 | -3.276 | 17.549 | | C |
| ATOM | 965 | | | B2009 | 16.931 | -5.091 | 17.257 | 1.00 14.49 | c |
| ATOM | 966 | | | B2009 | 16.666 | -4.783 | 15.777 | 1.00 15.47 | C |
| MOTA | 967 | C | | B2009 | 16.155 | -4.916 | 20.066 | 1.00 14.94 | 0 |
| ATOM | 968 | 0 | | B2009 | 16.090 | -6.145 | 20.190 | 1.00 14.51 | |
| MOTA | 969 | N | | B2010 | 15.115 | -4.111 | 20.318 | 1.00 15.66 | N C |
| ATOM | 970 | CA | | B2010 | 13.806 | -4.644 | 20.746 | 1.00 17.47 | c |
| ATOM | 971 | CB | | B2010 | 13.820 | -4.974 | 22.250 | 1.00 18.72 | |
| ATOM | 972 | CG | | B2010 | 12.474 | -5.527 | 22.757 | 1.00 19.74 | C |
| ATOM | 973 | | | B2010 | 11.670 | -4.747 | 23.311 | 1.00 21.08 | 0 |
| ATOM | 974 | | | B2010 | 12.214 | -6.740 | 22.593 | 1.00 19.62 | 0 |
| ATOM | 975 | C | | B2010 | 12.623 | -3.709 | 20.447 | 1.00 18.58 | C |
| ATOM | 976 | 0 | - | B2010 | 12.769 | -2.483 | 20.472 | 1.00 17.47 | 0 |
| MOTA | 977 | N | | B2011 | 11.465 | -4.304 | 20.148 | 1.00 19.97 | N |
| ATOM | 978 | CA | | B2011 | 10.224 | -3.558 | 19.874 | 1.00 22.59 | C |
| ATOM | 979 | CB | | B2011 | 9.666 | -3.817 | 18.459 | 1.00 23.44 | C |
| ATOM | 980 | | | B2011 | 8.532 | -2.831 | 18.167 | 1.00 24.17 | C |
| ATOM | 981 | | | B2011 | 10.752 | -3.688 | 17.411 | 1.00 23.83 | C |
| MOTA | 982 | | | B2011 | 10.368 | -4.350 | 16.110 | 1.00 24.58 | C |
| MOTA | 983 | С | | B2011 | 9.134 | -4.066 | 20.833 | 1.00 23.70 | C |
| ATOM | 984 | 0 | | B2011 | 9.039 | -5.271 | 21.078 | 1.00 23.87 | 0 |
| ATOM | 985 | N | | B2012 | 8.305 | -3.166 | 21.359 | 1.00 24.36 | N |
| ATOM | 986 | CA | | B2012 | 7.232 | -3.569 | 22.270 | 1.00 25.44 | C |
| ATOM | 987 | CB | | B2012 | 7.626 | -3.297 | 23.723 | 1.00 26.83 | C |
| MOTA | 988 | CG | | B2012 | 6.659 | -3.896 | 24.741 | 1.00 29.96 | C |
| MOTA | 989 | CD | GLU | B2012 | 6.806 | -5.408 | 24.892 | 1.00 32.18 | С |
| | | | | | | | | | |

| ATOM | 990 | OE1 | GLU | B2012 | 7.094 | -6.098 | 23.888 | 1.00 33.01 | 0 |
|------|--------------|----------|-----|----------------|----------------|----------------|--------|------------|---|
| ATOM | 991 | OE2 | GLU | B2012 | 6.617 | -5.908 | 26.024 | 1.00 33.41 | Ō |
| MOTA | 992 | С | | B2012 | 5.915 | -2.848 | 21.952 | 1.00 25.77 | Č |
| MOTA | 993 | 0 | | B2012 | 5.911 | -1.677 | 21.585 | 1.00 24.25 | Ō |
| ATOM | 994 | N | | B2013 | 4.800 | -3.563 | 22.089 | 1.00 26.07 | N |
| MOTA | 995 | CA | | B2013 | 3.483 | -2.997 | 21.806 | 1.00 26.79 | Ċ |
| ATOM | 996 | CB | | B2013 | 2.546 | -4.097 | 21.294 | 1.00 27.06 | Ċ |
| ATOM | 997 | CG | | B2013 | 3.025 | -4.777 | 20.014 | 1.00 27.29 | č |
| ATOM | 998 | CD | | B2013 | 2.147 | -5.943 | 19.607 | 0.05 27.19 | c |
| ATOM | 999 | OE1 | | B2013 | 0.920 | -5.750 | 19.479 | 0.05 27.19 | Ö |
| ATOM | 1000 | | | B2013 | 2.684 | -7.054 | 19.413 | 0.05 27.19 | 0 |
| ATOM | 1001 | C | | B2013 | 2.895 | -2.358 | 23.061 | 1.00 27.09 | c |
| ATOM | 1001 | 0 | | B2013 | 2.816 | -2.998 | 24.113 | 1.00 27.00 | 0 |
| ATOM | 1002 | N | | B2013 | 2.489 | -1.096 | 22.952 | 1.00 27.74 | N |
| ATOM | 1003 | | | B2014 | 1.915 | -0.383 | 24.088 | 1.00 27.74 | C |
| | | CA | | | | | 23.666 | 1.00 28.99 | C |
| ATOM | 1005 1006 | CB CG | | B2014 B2014 | 1.448 2.499 | 1.015 2.064 | 23.000 | 1.00 29.83 | C |
| ATOM | | | | B2014 | | | 22.863 | 1.00 30.49 | C |
| ATOM | 1007 | | | | 1.802 | 3.353 | | | |
| ATOM | 1008 | | | B2014 | 3.408 | 2.332 | 24.477 | 1.00 30.66 | C |
| ATOM | 1009 | С | | B2014 | 0.742 | -1.144 | 24.705 | 1.00 29.62 | C |
| ATOM | 1010 | 0 | | B2014 | 0.614 | -1.209 | 25.924 | 1.00 28.92 | 0 |
| ATOM | 1011 | N | | B2015 | -0.103 | -1.723 | 23.855 | 1.00 30.68 | N |
| MOTA | 1012 | CA | | B2015 | -1.273 | -2.468 | 24.312 | 1.00 31.89 | С |
| MOTA | 1013 | CB | | B2015 | -2.062 | -2.992 | 23.106 | 1.00 31.63 | C |
| ATOM | 1014 | С | | B2015 | -0.942 | -3.624 | 25.256 | 1.00 32.68 | C |
| ATOM | 1015 | 0 | | B2015 | -1.705 | -3.913 | 26.180 | 1.00 32.95 | 0 |
| ATOM | 1016 | N | | B2016 | 0.192 | -4.282 | 25.026 | 1.00 32.98 | N |
| ATOM | 1017 | CA | | B2016 | 0.599 | -5.409 | 25.861 | 1.00 33.69 | C |
| ATOM | 1018 | CB | | B2016 | 1.758 | -6.157 | 25.205 | 1.00 34.30 | C |
| ATOM | 1019 | OG | | B2016 | 1.360 | -6.697 | 23.955 | 1.00 36.37 | 0 |
| MOTA | 1020 | С | | B2016 | 0.993 | -4.981 | 27.271 | 1.00 33.62 | С |
| ATOM | 1021 | 0 | | B2016 | 0.707 | -5.680 | 28.242 | 1.00 33.30 | 0 |
| ATOM | 1022 | N | | B2017 | 1.656 | -3.835 | 27.384 | 1.00 33.85 | N |
| ATOM | 1023 | CA | | B2017 | 2.056 | -3.339 | 28.694 | 1.00 34.29 | С |
| ATOM | 1024 | CB | | B2017 | 2.995 | -2.115 | 28.571 | 1.00 34.08 | С |
| ATOM | 1025 | | | B2017 | 3.350 | -1.588 | 29.958 | 1.00 33.83 | С |
| MOTA | 1026 | | | B2017 | 4.264 | -2.501 | 27.800 | 1.00 33.75 | С |
| ATOM | 1027 | | | B2017 | 5.080 | -3.611 | 28.449 | 1.00 33.98 | C |
| ATOM | 1028 | С | | B2017 | 0.802 | -2.932 | 29.474 | 1.00 35.14 | С |
| ATOM | 1029 | 0 | | B2017 | 0.714 | -3.143 | 30.683 | 1.00 34.67 | 0 |
| ATOM | 1030 | N | | B2018 | -0.172 | -2.362 | 28.770 | 1.00 36.36 | N |
| MOTA | 1031 | CA | | B2018 | -1.414 | -1.925 | 29.402 | 1.00 37.92 | С |
| ATOM | 1032 | СВ | | B2018 | -2.292 | -1.189 | 28.386 | 1.00 38.65 | C |
| ATOM | 1033 | CG | | B2018 | -1.548 | -0.122 | 27.599 | 1.00 40.03 | С |
| ATOM | 1034 | CD | | B2018 | -2.462 | 0.705 | | 1.00 41.09 | С |
| MOTA | 1035 | | | B2018 | -3.463 | 0.148 | 26.216 | 1.00 41.60 | 0 |
| ATOM | 1036 | OE2 | | B2018 | -2.172 | 1907 | 26.510 | 1.00 41.15 | 0 |
| ATOM | 1037 | С | | B2018 | -2.189 | -3.093 | 30.011 | 1.00 38.32 | С |
| MOTA | 1038 | 0 | | B2018 | -2.697 | -2.993 | 31.129 | 1.00 39.05 | 0 |
| MOTA | 1039 | N | | B2019 | -2.281 | -4.198 | 29.278 | 1.00 38.71 | N |
| MOTA | 1040 | CA | | B2019 | | -5.375 | 29.771 | 1.00 39.10 | С |
| MOTA | 1041 | CB | | B2019 | -2.996 | -6.476 | 28.709 | 1.00 39.02 | С |
| ATOM | 1042 | OG | | B2019 | -3.734 | -6.082 | 27.568 | 1.00 39.39 | 0 |
| MOTA | 1043 | С | | B2019 | -2.332 | -5.903 | 31.044 | 1.00 39.56 | С |
| MOTA | 1044 | 0 | | B2019 | -3.013 | -6.228 | 32.016 | 1.00 39.07 | 0 |
| ATOM | 1045 | N | | B2020 | -1.004 | -5.983 | 31.031 | 1.00 39.92 | N |
| MOTA | 1046 | CA | ALA | B2020 | -0.253 | -6.471 | 32.182 | 1.00 40.75 | С |

| ATOM | 1047 | СВ | ALA | B2020 | 1.240 | -6.474 | 31.866 | 1.00 39.96 | | С |
|------|------|--------|-----|-------|----------------------|---------------------|--------|------------|---|---|
| ATOM | 1048 | С | | B2020 | -0.531 | -5.614 | 33.415 | 1.00 41.51 | | С |
| ATOM | 1049 | 0 | ALA | B2020 | -0.584 | -6.122 | 34.535 | 1.00 41.34 | | 0 |
| ATOM | 1050 | N | | B2021 | -0.704 | -4.314 | 33.202 | 1.00 42.82 | | N |
| ATOM | 1051 | CA | | B2021 | -0.985 | -3.390 | 34.295 | 1.00 44.39 | | С |
| ATOM | 1052 | СВ | | B2021 | -0.767 | -1.922 | 33.855 | 1.00 44.31 | | C |
| ATOM | 1053 | | | B2021 | -1.303 | -0.971 | 34.913 | 1.00 44.07 | | Ċ |
| ATOM | 1053 | | | B2021 | 0.718 | -1.663 | 33.627 | 1.00 44.22 | | č |
| ATOM | 1055 | C· | | B2021 | -2.424 | -3.555 | 34.787 | 1.00 45.72 | | C |
| | 1056 | | | B2021 | -2.673 | -3.604 | 35.992 | 1.00 45.74 | | Ö |
| MOTA | | O N | | B2021 | -3.365 | -3.642 | 33.851 | 1.00 47.27 | | N |
| ATOM | 1057 | | | | | | | 1.00 47.27 | | C |
| ATOM | 1058 | CA | | B2022 | -4.776 | -3.801 | 34.191 | 1.00 49.02 | | C |
| ATOM | 1059 | CB | | B2022 | -5.661 | -3.833 | 32.919 | | | |
| ATOM | 1060 | | | B2022 | -5.482 | -2.619 | 32.177 | 1.00 49.29 | | 0 |
| ATOM | 1061 | CG2 | | B2022 | -7.134 | -3.968 ⁻ | 33.293 | 1.00 49.42 | | C |
| ATOM | 1062 | С | | B2022 | -4.988 | -5.093 | 34.977 | 1.00 49.61 | | C |
| ATOM | 1063 | 0 | | B2022 | -5.953 | -5.225 | 35.733 | 1.00 49.90 | | 0 |
| ATOM | 1064 | N | | B2023 | -4.077 | -6.043 | 34.794 | 1.00 50.61 | | N |
| MOTA | 1065 | CA | | B2023 | -4.152 | -7.325 | 35.484 | 1.00 51.35 | | С |
| ATOM | 1066 | CB | | B2023 | -3.028 | -8.245 | 35.009 | 1.00 52.09 | | С |
| MOTA | 1067 | CG | ARG | B2023 | -3.416 | -9.710 | 34.907 | 1.00 53.02 | | С |
| MOTA | 1068 | CD | ARG | B2023 | -3.676 | -10.103 | 33.461 | 1.00 54.10 | | С |
| MOTA | 1069 | NE | ARG | B2023 | -2.492 | -9.895 | 32.628 | 1.00 54.73 | | N |
| ATOM | 1070 | CZ | ARG | B2023 | -2.419 | -10.194 | 31.334 | 1.00 55.21 | | C |
| ATOM | 1071 | NH1 | ARG | B2023 | | -10.720 | 30.710 | 1.00 55.43 | * | N |
| ATOM | 1072 | NH2 | ARG | B2023 | -1.296 | -9.967 | 30.663 | 1.00 55.24 | | N |
| ATOM | 1073 | С | ARG | B2023 | -4 ¹ .025 | -7.093 | 36.989 | 1.00 51.64 | | С |
| ATOM | 1074 | 0 | ARG | B2023 | -4.448 | -7.924 | 37.794 | 1.00 51.91 | | 0 |
| ATOM | 1075 | N | HIS | B2024 | -3.428 | -5.960 | 37.354 | 1.00 51.80 | | N |
| ATOM | 1076 | CA | HIS | B2024 | -3.242 | -5.575 | 38.753 | 1.00 51.59 | | С |
| ATOM | 1077 | CB | | B2024 | -4.586 | -5.645 | 39.491 | 1.00 52.56 | | С |
| ATOM | 1078 | CG | | B2024 | -4.528 | -5.165 | 40.908 | 1.00 53.50 | | С |
| ATOM | 1079 | | | B2024 | -4.815 | -5.791 | 42.074 | 1.00 53.85 | | С |
| ATOM | 1080 | | | B2024 | -4.142 | -3.886 | 41.245 | 1.00 53.73 | | N |
| ATOM | 1081 | | | B2024 | -4.195 | -3.743 | 42.557 | 1.00 54.11 | | C |
| MOTA | 1082 | | | B2024 | -4.601 | -4.885 | 43.084 | 1.00 54.34 | | N |
| MOTA | 1083 | C | | B2024 | -2.207 | -6.427 | 39.490 | 1.00 50.92 | | С |
| ATOM | 1084 | Ö | | B2024 | -1.802 | -6.100 | 40.607 | 1.00 51.09 | | Ö |
| ATOM | 1085 | N | | B2025 | -1.777 | -7.511 | 38.853 | 1.00 49.85 | | N |
| ATOM | 1086 | CA | | B2025 | -0.805 | -8.436 | 39.429 | 1.00 48.60 | | C |
| ATOM | 1087 | CB | | B2025 | -0.133 | -9.231 | 38.309 | 1.00 49.70 | | C |
| ATOM | 1088 | CG | | B2025 | -1.109 | -9.812 | 37.300 | 1.00 50.84 | | Č |
| | | CD | | B2025 | | -10.676 | 36.255 | 1.00 51.43 | | č |
| ATOM | 1089 | | - | B2025 | | -11.754 | 36.617 | 1.00 52.08 | | 0 |
| MOTA | 1090 | | | | | | | 1.00 52.00 | | Ö |
| MOTA | 1091 | OE2 | | B2025 | | -10.276 | 35.073 | | | |
| ATOM | 1092 | C | | B2025 | 0.274 | -7.788 | 40.301 | 1.00 47.18 | | C |
| ATOM | 1093 | 0 | | B2025 | 0.636 | -8.322 | 41.350 | 1.00 47.28 | • | 0 |
| ATOM | 1094 | Ν. | | B2026 | 0.779 | -6.638 | 39.864 | 1.00 45.23 | | N |
| ATOM | 1095 | | | B2026 | 1.832 | -5.953 | 40.598 | 1.00 42.17 | | С |
| ATOM | 1096 | C | | B2026 | 3.021 | -5.830 | 39.663 | 1.00 39.71 | | С |
| ATOM | 1097 | 0 | | B2026 | 4.185 | -5.914 | 40.066 | 1.00 39.77 | | 0 |
| ATOM | 1098 | N | | B2027 | 2.695 | -5.632 | 38.392 | 1.00 37.19 | | N |
| MOTA | 1099 | ÇA | | B2027 | 3.667 | -5.509 | 37.315 | 1.00 34.55 | | C |
| MOTA | 1100 | CB | | B2027 | 2.922 | -5.189 | 36.014 | 1.00 34.52 | | C |
| MOTA | 1101 | CG | | B2027 | 3.752 | - 5.355 | 34.777 | 1.00 34.13 | | С |
| ATOM | 1102 | | | B2027 | 4.207 | | 34.393 | 1.00 34.08 | | С |
| MOTA | 1103 | CD2 | PHE | B2027 | 4.067 | -4.258 | 33.986 | 1.00 34.08 | | С |
| | | | | | | | | | | |

| ATOM | 1104 | CE1 | PHE | B2027 | 4.963 | -6.776 | 33.237 | 1.00 34.11 | С |
|--------------|--------------|-----|-----|----------------|----------------|----------|------------------|--------------------------|--------|
| MOTA | 1105 | CE2 | PHE | B2027 | 4.825 | -4.409 | 32.824 | 1.00 34.27 | С |
| MOTA | 1106 | CZ | PHE | B2027 | 5.274 | -5.670 | 32.449 | 1.00 34.06 | С |
| ATOM | 1107 | С | PHE | B2027 | 4.755 | -4.459 | 37.559 | 1.00 32.71 | C, |
| MOTA | 1108 | 0 | PHE | B2027 | 5.933 | -4.794 | 37.676 | 1.00 31.86 | 0 |
| MOTA | 1109 | N | ALA | B2028 | 4.352 | -3.192 | 37.631 | 1.00 30.82 | N |
| ATOM | 1110 | CA | ALA | B2028 | 5.284 | -2.082 | 37.831 | 1.00 29.20 | C |
| ATOM | 1111 | CB | ALA | B2028 | 4.506 | -0.787 | 38.047 | 1.00 29.12 | С |
| ATOM | 1112 | С | ALA | B2028 | 6.290 | -2.269 | 38.966 | 1.00 28.66 | С |
| ATOM | 1113 | 0 | ALA | B2028 | 7.451 | -1.884 | 38.836 | 1.00 27.76 | 0 |
| MOTA | 1114 | N | LYS | B2029 | 5.846 | -2.853 | 40.075 | 1.00 27.74 | И |
| MOTA | 1115 | CA | LYS | B2029 | 6.718 | • | 41.226 | 1.00 27.62 | C |
| MOTA | 1116 | CB | | B2029 | 5.899 | | 42.423 | 1.00 27.96 | С |
| MOTA | 1117 | CG | LYS | B2029 | 5.853 | | 43.584 | 1.00 28.74 | С |
| ATOM | 1118 | CD | LYS | B2029 | 7.247 | | 44.131 | 0.05 28.50 | С |
| ATOM | 1119 | CE | LYS | B2029 | 7.204 | | 45.343 | 0.05 28.61 | C |
| MOTA | 1120 | NZ | | B2029 | 6.454 | | 46.474 | 0.05 28.56 | . N |
| ATOM | 1121 | С | | B2029 | 7.864 | | 40.969 | 1.00 27.09 | С |
| MOTA | 1122 | 0 | | B2029 | 8.937 | | 41.555 | 1.00 27.52 | 0 |
| ATOM | 1123 | N | | B2030 | 7.642 | | 40.099 | 1.00 25.99 | N |
| ATOM | 1124 | CA | | B2030 | 8.682 | | 39.803 | 1.00 24.71 | С |
| ATOM | 1125 | CB | | B2030 | 8.048 | | 39.465 | 1.00 25.36 | С |
| ATOM | 1126 | CG | | B2030 | 7.303 | | 40.631 | 0.05 25.04 | C |
| ATOM | 1127 | | | B2030 | 6.804 | | 40.291 | 0.05 25.09 | C |
| ATOM | 1128 | NE | | B2030 | | -10.015 | 41.430 | 0.05 25.02 | N |
| MOTA | 1129 | CZ | | B2030 | | -11.249 | 41.421 | 0.05 25.00 | C |
| MOTA | 1130 | | | B2030 | | -11.996 | 40.329 | 0.05 24.97 | N |
| MOTA | 1131 | | | B2030 | | -11.739 | 42.506 | 0.05 24.97 | N |
| ATOM | 1132 | C | | B2030 | 9.616 | | 38.674 | 1.00.23.43 | C |
| ATOM | 1133 | 0 | | B2030 | 10.763 | | 38.613 | 1.00 22.95 | 0 |
| ATOM | 1134 | N | | B2031 | 9.131 | | 37.797 | 1.00 22.08 | N C |
| ATOM | 1135 | CA | | B2031 | 9.924 | | 36.665 | 1.00 20.91 | C |
| ATOM | 1136 | CB | | B2031 | 8.998 9.804 | | 35.447 34.307 | 1.00 21.66 1.00 21.12 | C |
| ATOM ATOM | 1137 1138 | | | B2031 B2031 | 8.311 | | 34.961 | 1.00 21.12 | C |
| ATOM | 1139 | CGZ | | B2031 | 10.806 | | 36.946 | 1.00 20.08 | Ċ |
| ATOM | 1140 | 0 | | B2031 | 11.891 | | 36.362 | 1.00 18.87 | 0 |
| ATOM | 1141 | N | | B2032 | 10.362 | | 37.851 | 1.00 18.43 | N |
| ATOM | 1142 | CA | | B2032 | 11.093 | | 38.170 | 1.00 18.33 | C |
| ATOM | 1143 | CB | | B2032 | 10.123 | | 38.094 | 1.00 18.11 | Ċ |
| ATOM | 1144 | CG | | B2032 | 9.264 | | 36.836 | 1.00 17.77 | C |
| ATOM | 1145 | | | B2032 | 8.288 | | 37.095 | 1.00 18.63 | C |
| ATOM | 1146 | | | B2032 | 10.141 | | 35.642 | 1.00 18.26 | С |
| ATOM | 1147 | С | | B2032 | 11.809 | | 39.537 | 1.00 18.11 | C |
| ATOM | 1148 | 0 | LEU | B2032 | 11.313 | 3 -1.351 | 40.528 | 1.00 17.53 | 0 |
| ATOM | 1149 | N | THR | B2033 | 12.964 | -0.133 | 39.589 | 1.00 17.46 | N |
| ATOM | 1150 | CA | THR | B2033 | 13.70 | | 40.848 | 1.00 17.07 | С |
| ATOM | 1151 | CB | THR | B2033 | 15.178 | 0.466 | 40.617 | 1.00 17.19 | C |
| ATOM | 1152 | OG1 | THR | B2033 | 15.199 | 1.760 | 39.996 | 1.00 17.05 | 0 |
| ATOM | 1153 | CG2 | THR | B2033 | 15.919 | 0.544 | 39.733 | 1.00 15.96 | C |
| ATOM | 1154 | С | | B2033 | 13.010 | | 41.686 | 1.00 17.66 | . C |
| MOTA | 1155 | 0 | | B2033 | 12.042 | | 41.234 | 1.00 17.87 | 0 |
| MOTA | 1156 | N | | B2034 | 13.50 | | 42.896 | 1.00 17.54 | N |
| MOTA | 1157 | CA | | B2034 | 12.88 | | 43.757 | 1.00 18.74 | C |
| MOTA | 1158 | CB | | B2034 | 13.56 | | 45.123 | 1.00 18.99 | C |
| ATOM | 1159 | C | | B2034 | 12.92 | | 43.145 | 1.00 18.65 | С |
| MOTA | 1160 | 0 | ALA | B2034 | 11.93 | 4.503 | 43.188 | 1.00 18.77 | . 0 |

| ATOM | 1161 | N | 7 =11 | B2035 | | 14.066 | 4.148 | 42.572 | 1.00 18.26 | N |
|------|------|-----|-------|---------|---|--------|----------------|------------------|--------------------------|-----|
| ATOM | 1162 | CA | | B2035 | | 14.216 | 5.470 | 41.962 | 1.00 19.09 | C |
| ATOM | 1163 | CB | | B2035 | | 15.697 | | 41.665 | 1.00 20.60 | Ċ |
| ATOM | 1164 | | | B2035 | | 16.154 | 7.182 | 41.435 | 1.00 22.12 | č |
| | 1165 | | | B2035 | | 15.976 | 8.015 | 42.714 | 1.00 23.52 | Č |
| ATOM | | | | B2035 | | 17.618 | 7.173 | 41.031 | 1.00 24.30 | c |
| ATOM | 1166 | | | B2035 | | 13.383 | 5.610 | 40.680 | 1.00 18.93 | c |
| ATOM | 1167 | C | | | | | 6.670 | 40.430 | 1.00 10.55 | 0 |
| ATOM | 1168 | 0 | | B2035 | | 12.801 | | | 1.00 19.57 | И |
| ATOM | 1169 | N | | B2036 | | 13.333 | 4.559 | 39.858 38.626 | 1.00 18.35 | C |
| ATOM | 1170 | CA | | B2036 | | 12.533 | 4.604 3.327 | | 1.00 17.51 | C |
| MOTA | 1171 | CB | | B2036 | | 12.733 | | 37.784 | | C |
| ATOM | 1172 | CG | | B2036 | | 14.085 | 3.215 | 37.042 | 1.00 15.99 1.00 16.12 | C |
| MOTA | 1173 | CD | | B2036 | | 14.300 | 1.848 | 36.391 | | 0 |
| ATOM | 1174 | | | B2036 | | 15.007 | 1.777 | 35.361 | 1.00 15.21 | |
| ATOM | 1175 | | | B2036 | | 13.781 | 0.836 | 36.911 | 1.00 15.16 | 0 |
| MOTA | 1176 | C | | B2036 | | 11.039 | 4.744 | 38.982 | 1.00 19.23 | С |
| ATOM | 1177 | 0 | | B2036 | | 10.290 | 5.440 | 38.296 | 1.00 19.60 | 0 |
| ATOM | 1178 | N | | B2037 | | 10.616 | 4.074 | 40.051 | 1.00 19.86 | N |
| MOTA | 1179 | CA | | B2037 | | 9.219 | 4.123 | 40.501 | 1.00 21.88 | C |
| MOTA | 1180 | CB | | B2037 | | 9.008 | 3.086 | 41.615 | 1.00 22.85 | C |
| ATOM | 1181 | CG | | B2037 | | 7.623 | 3.055 | 42.236 | 1.00 25.86 | C |
| ATOM | 1182 | SD | | B2037 | | 6.356 | 2.391 | 41.143 | 1.00 28.53 | S |
| ATOM | 1183 | CE | | B2037 | | 6.759 | 0.626 | 41.201 | 1.00 27.97 | С |
| MOTA | 1184 | С | | B2037 | | 8.834 | 5.528 | 41.000 | 1.00 22.03 | С |
| MOTA | 1185 | 0 | | B2037 | | 7.716 | 6.006 | 40.772 | 1.00 22.35 | 0 |
| MOTA | 1186 | N | | B2038 | | 9.759 | 6.187 | 41.687 | 1.00 22.54 | N |
| MOTA | 1187 | CA | GLU | B2038 | | 9.501 | 7.528 | 42.194 | 1.00 23.34 | С |
| ATOM | 1188 | CB | GLU | B2038 | | 10.663 | 7.973 | 43.101 | 1.00 23.49 | C |
| MOTA | 1189 | CG | | B2038 | | 10.475 | 7.496 | 44.550 | 1.00 24.52 | C |
| MOTA | 1190 | CD | GLU | B2038 | | 11.772 | 7.284 | 45.326 | 1.00 25.50 | С |
| ATOM | 1191 | OE1 | GLU | B2038 | | 12.785 | 7.962 | 45.036 | 1.00 25.67 | · O |
| MOTA | 1192 | OE2 | GLU | B2038 | | 11.765 | 6.439 | 46.251 | 1.00 25.94 | 0 |
| MOTA | 1193 | С | GLU | B2038 | | 9.252 | 8.513 | 41.046 | 1.00 23.18 | С |
| MOTA | 1194 | 0 | | B2038 | | 8.512 | 9.482 | 41.200 | 1.00 23.42 | 0 |
| MOTA | 1195 | N | ARG | B2039 | | 9.854 | 8.250 | 39.888 | 1.00 23.18 | N |
| ATOM | 1196 | CA | ARG | B2039 | | 9.659 | 9.097 | 38.713 | 1.00 23.42 | С |
| MOTA | 1197 | CB | ARG | B2039 | | 10.801 | 8.888 | 37.710 | 1.00 24.21 | C |
| MOTA | 1198 | CG | | B2039 | | 10.566 | 9.517 | 36.338 | 1.00 24.82 | C |
| ATOM | 1199 | CD | | B2039 | | 10.414 | 11.027 | 36.415 | 0.05 24.52 | C |
| MOTA | 1200 | ΝE | ARG | B2039 | ٠ | 10.169 | 11.609 | 35.099 | 0.05 24.58 | N |
| MOTA | 1201 | CZ | | B2039 | | 9,995 | 12.908 | 34.873 | 0.05 24.54 | С |
| MOTA | 1202 | | | B2039 | | 9.776 | 13.344 | 33.640 | 0.05 24.55 | N |
| ATOM | 1203 | | | B2039 | | 10.039 | | . 35.879 | 0.05 24.55 | N |
| ATOM | 1204 | С | ARG | B2039 | | 8.323 | 8.738 | 38.057 | 1.00 22.97 | C |
| ATOM | 1205 | 0 | | B2039 | | 7.591 | 9.614 | 37.594 | 1.00 23.62 | 0 |
| MOTA | 1206 | N | | B2040 | | 8.015 | 7.443 | 38.037 | 1.00 22.59 | N |
| MOTA | 1207 | CA | | B2040 | | 6.777 | 6.914 | 37.456 | 1.00 23.04 | C |
| MOTA | 1208 | CB | | B2040 | | 6.769 | 5.381 | 37.598 | 1.00 23.27 | C |
| ATOM | 1209 | CG | | B2040 | | 5.520 | 4.705 | 37.082 | 1.00 24.49 | C |
| ATOM | 1210 | | | B2040 | | 5.270 | 4.604 | 35.716 | 1.00 24.75 | c |
| MOTA | 1211 | | | B2040 | | 4.611 | 4.125 | 37.971 | 1.00 24.92 | c |
| MOTA | 1212 | | | B2040 | | 4.135 | 3.930 | 35.240 | 1.00 25.22 | c |
| MOTA | 1213 | | | B2040 | | 3.473 | 3.451 | 37.509 | 1.00 24.72 | C |
| MOTA | 1214 | CZ | | B2040 | | 3.236 | 3.353 | 36.139 | 1.00 25.48 | C |
| MOTA | 1215 | С | | B2040 | | 5.529 | 7.506 | 38.126 | 1.00 23.15 | C |
| ATOM | 1216 | 0 | | B2040 | | 4.558 | 7.841 | 37.448 | 1.00 22.73 | 0 |
| MOTA | 1217 | N | THE | R B2041 | | 5.559 | 7.636 | 39.452 | 1.00 23.63 | N |
| | | | | | | | | | | |

| MOTA | 1218 | CA | THR | B2041 | 4.407 | 8.165 | 40.186 | 1.00 25.06 | С |
|------|------|-----|-----|-------|--------|--------|---------|------------|-----|
| ATOM | 1219 | CB | THR | B2041 | 4.487 | 7.819 | 41.701 | 1.00 24.62 | С |
| ATOM | 1220 | OG1 | THR | B2041 | 5.710 | 8.322 | 42.250 | 1.00 24.25 | 0 |
| ATOM | 1221 | CG2 | THR | B2041 | 4.421 | 6.311 | 41.910 | 1.00 24.17 | С |
| ATOM | 1222 | С | | B2041 | 4.156 | 9.669 | 40.050 | 1.00 25.84 | С |
| ATOM | 1223 | 0 | | B2041 | 3.089 | 10.155 | 40.442 | 1.00 26.22 | 0 |
| ATOM | 1224 | N | | B2042 | 5.119 | 10.412 | 39.508 | 1.00 27.24 | N |
| ATOM | 1225 | CA | | B2042 | 4.939 | 11.856 | 39.346 | 1.00 28.70 | C |
| ATOM | 1226 | CB | | B2042 | 6.256 | 12.605 | 39.605 | 1.00 29.90 | č |
| ATOM | 1227 | OG | | B2042 | 7.260 | 12.270 | 38.658 | 1.00 31.49 | Ö |
| ATOM | 1228 | C | | B2042 | 4.404 | 12.214 | 37.959 | 1.00 29.44 | c |
| ATOM | 1229 | 0 | | B2042 | 4.245 | 13.392 | 37.632 | 1.00 28.96 | 0 |
| ATOM | 1230 | N | | B2042 | 4.127 | 11.192 | 37.151 | 1.00 29.93 | Ŋ |
| ATOM | 1231 | CA | | B2043 | 3.598 | 11.379 | 35.797 | 1.00 30.98 | C |
| ATOM | 1231 | CB | | B2043 | 4.466 | 10.622 | 34.779 | 1:00 30.83 | č |
| ATOM | 1232 | CG | | B2043 | 5.925 | 11.061 | 34.614 | 1.00 30.66 | c |
| | | | | | 6.690 | 10.037 | 33.778 | 1.00 30.00 | C |
| ATOM | 1234 | | | B2043 | 5.970 | 12.431 | 33.776 | 1.00 31.31 | C |
| ATOM | 1235 | | | B2043 | | | | 1.00 31.30 | c |
| MOTA | 1236 | С | | B2043 | 2.160 | 10.864 | 35.712 | | |
| MOTA | 1237 | 0 | | B2043 | 1.711 | 10.106 | 36.573 | 1.00 31.45 | 0 |
| ATOM | 1238 | N | | B2044 | 1.440 | 11.264 | 34.668 | 1.00 33.21 | N |
| MOTA | 1239 | CA | | B2044 | 0.059 | 10.820 | 34.497 | 1.00 34.53 | С |
| ATOM | 1240 | CB | | B2044 | -0.904 | 11.853 | 35.100 | 1.00 35.00 | C |
| MOTA | 1241 | CG | | B2044 | -2.362 | 11.415 | 35.118 | 0.05 34.86 | C |
| ATOM | 1242 | CD | | B2044 | -3.267 | 12.481 | 35.714 | 0.05 34.96 | C |
| ATOM | 1243 | CE | | B2044 | -4.718 | 12.025 | 35.718 | 0.05 34.95 | C |
| ATOM | 1244 | NZ | | B2044 | -5.625 | 13.056 | 36.293 | 0.05 35.07 | N |
| ATOM | 1245 | С | | B2044 | -0.311 | 10.580 | 33.035 | 1.00 35.45 | C |
| ATOM | 1246 | 0 | | B2044 | 0.422 | 10.960 | 32.121 | 1.00 35.43 | 0 |
| ATOM | 1247 | N | | B2045 | -1.454 | 9.934 | 32.829 | 1.00 36.33 | N |
| ATOM | 1248 | CA | GLY | B2045 | -1.940 | 9.671 | 31.488 | 1.00 37.45 | С |
| ATOM | 1249 | С | | B2045 | -1.031 | 8.869 | 30.579 | 1.00 38.02 | С |
| ATOM | 1250 | 0 | GLY | B2045 | -0.215 | 8.065 | 31.03,6 | 1.00 38.35 | 0 |
| ATOM | 1251 | N | ARG | B2046 | -1.187 | 9.099 | 29.279 | 1.00 38.11 | N |
| MOTA | 1252 | CA | ARG | B2046 | -0.414 | 8.409 | 28.250 | 1.00 38.00 | С |
| ATOM | 1253 | CB | ARG | B2046 | -0.718 | 9.026 | 26.882 | 1.00 38.22 | С |
| ATOM | 1254 | CG | ARG | B2046 | 2.203 | 9.241 | 26.635 | 0.05 38.32 | С |
| ATOM | 1255 | CD | ARG | B2046 | -2.469 | 9.951 | 25.319 | 0.05 38.47 | С |
| ATOM | 1256 | NE | ARG | B2046 | -2.193 | 9.103 | 24.164 | 0.05 38.58 | N |
| MOTA | 1257 | CZ | ARG | B2046 | -2.418 | 9.462 | 22.904 | 0.05 38.64 | С |
| ATOM | 1258 | NH1 | ARG | B2046 | -2.138 | 8.626 | 21.915 | 0.05 38.67 | N |
| MOTA | 1259 | NH2 | ARG | B2046 | -2.925 | 10.657 | 22.633 | 0.05 38.67 | N |
| MOTA | 1260 | С | ARG | B2046 | 1.083 | 8.472 | 28.516 | 1.00 37.79 | С |
| ATOM | 1261 | Ο. | ARG | B2046 | 1.809 | 7.514 | 28.262 | 1.00 37.64 | 0 |
| ATOM | 1262 | N | ARG | B2047 | 1.534 | | 29.031 | | N |
| MOTA | 1263 | CA | ARG | B2047 | 2.945 | 9.827 | 29.327 | 1.00 36.86 | С |
| MOTA | 1264 | CB | ARG | B2047 | 3.139 | 11262 | 29.824 | 1.00 38.35 | С |
| ATOM | 1265 | CG | ARG | B2047 | 4.529 | 11.834 | 29.622 | 1.00 40.01 | С |
| ATOM | 1266 | CD | ARG | B2047 | 4.591 | 13.258 | 30.156 | 1.00 41.52 | C |
| MOTA | 1267 | NE | ARG | B2047 | 5.880 | 13.894 | 29.903 | 1.00 43.12 | N |
| ATOM | 1268 | CZ | | B2047 | 6.276 | 15.030 | 30.471 | 1.00 44.06 | С |
| ATOM | 1269 | NH1 | ARG | B2047 | 7.467 | 15.539 | 30.180 | 1.00 44.67 | N |
| ATOM | 1270 | | | B2047 | 5.486 | 15.654 | 31.336 | 1.00 44.50 | N |
| ATOM | 1271 | С | | B2047 | 3.460 | 8.826 | 30.368 | | С |
| ATOM | 1272 | 0 | | B2047 | 4.631 | 8.454 | 30.354 | 1.00 34.93 | 0 |
| ATOM | 1273 | N | | B2048 | 2.578 | 8.388 | 31.263 | 1.00 34.21 | · N |
| MOTA | 1274 | CA | | B2048 | 2.947 | 7.433 | 32.305 | 1.00 32.54 | С |
| | | | | | | | | | |

| ATOM | 1275 | CB | GLN | B2048 | 1.866 | 7.413 | 33.396 | 1.00 33.03 | С |
|------|------|-----------|-----|-------|---------|--------|--------|------------|---|
| ATOM | 1276 | CG | GLN | B2048 | 2.203 | 6.564 | 34.616 | 1.00 32.53 | С |
| MOTA | 1277 | CD | GLN | B2048 | 1.203 | 6.741 | 35.751 | 1.00 33.31 | С |
| MOTA | 1278 | OE1 | GLN | B2048 | 0.009 | 6.499 | 35.586 | 1.00 32.97 | 0 |
| ATOM | 1279 | NE2 | GLN | B2048 | 1.694 | 7.164 | 36.914 | 1.00 33.17 | N |
| ATOM | 1280 | С | | B2048 | 3.161 | 6.021 | 31.740 | 1.00 31.47 | С |
| ATOM | 1281 | 0 | | B2048 | 4.119 | 5.340 | 32.106 | 1.00 31.22 | 0 |
| ATOM | 1282 | N | | B2049 | . 2.269 | 5.589 | 30.852 | 1.00 29.87 | N |
| ATOM | 1283 | CA | | B2049 | 2.366 | 4.266 | 30.233 | 1.00 28.47 | С |
| ATOM | 1284 | CB | | B2049 | 1.087 | 3.936 | 29.417 | 1.00 28.92 | С |
| ATOM | 1285 | | | B2049 | 1.263 | 2.627 | 28.667 | 1.00 29.21 | С |
| ATOM | 1286 | | | B2049 | -0.130 | 3.858 | 30.346 | 1.00 29.32 | С |
| ATOM | 1287 | | | B2049 | -0.118 | 2.675 | 31.305 | 1.00 28.99 | C |
| ATOM | 1288 | C | | B2049 | 3.577 | 4.191 | 29.292 | 1.00 27.84 | С |
| ATOM | 1289 | o | | B2049 | 4.172 | 3.127 | 29.116 | 1.00 27.30 | Ō |
| ATOM | 1290 | N | | B2049 | 3.933 | 5.321 | 28.688 | 1.00 26.72 | N |
| ATOM | 1291 | CA | | B2050 | 5.073 | 5.373 | 27.774 | 1.00 26.84 | C |
| ATOM | 1291 | CB | | B2050 | 5.060 | 6.692 | 26.985 | 1.00 27.77 | Č |
| | | | | | 6.298 | 6.973 | 26.119 | 1.00 30.05 | c |
| ATOM | 1293 | CG | | B2050 | 6.456 | 6.027 | 24.927 | 1.00 30.33 | Ċ |
| ATOM | 1294 | CD CE1 | | B2050 | | | 24.262 | 1.00 31.34 | 0 |
| ATOM | 1295 | | | B2050 | 5.443 | 5.718 | | 1.00 32.49 | 0 |
| ATOM | 1296 | | | B2050 | 7.603 | 5.610 | 24.643 | 1.00 31.18 | č |
| ATOM | 1297 | С | | B2050 | 6.397 | 5.223 | 28.520 | | 0 |
| MOTA | 1298 | 0 | | B2050 | 7.339 | 4.621 | 27.994 | 1.00 24.70 | Ŋ |
| MOTA | 1299 | N | | B2051 | 6.471 | 5.767 | 29.737 | 1.00 23.32 | C |
| MOTA | 1300 | CA | | B2051 | 7.696 | 5.675 | 30.537 | 1.00 21.39 | |
| MOTA | 1301 | CB | | B2051 | 7.576 | 6.526 | 31.821 | 1.00 21.45 | C |
| MOTA | 1302 | CG | | B2051 | 8.819 | 6.522 | 32.712 | 1.00 20.60 | C |
| MOTA | 1303 | | | B2051 | 8.974 | 5.577 | 33.728 | 1.00 20.47 | C |
| ATOM | 1304 | | | B2051 | 10.128 | 5.547 | 34.526 | 1.00 20.26 | C |
| MOTA | 1305 | | | B2051 | 9.852 | 7.444 | 32.512 | 1.00 20.44 | C |
| MOTA | 1306 | | TYR | B2051 | 11.012 | 7.420 | 33.302 | 1.00 20.69 | C |
| ATOM | 1307 | CZ | TYR | B2051 | 11.141 | 6.469 | 34.306 | 1.00 20.69 | С |
| ATOM | 1308 | OH | | B2051 | 12.277 | 6.449 | 35.094 | 1.00 21.32 | 0 |
| ATOM | 1309 | С | | B2051 | 7.978 | 4.212 | 30.885 | 1.00 20.75 | C |
| MOTA | 1310 | 0 | TYR | B2051 | 9.085 | 3.718 | 30.658 | 1.00 19.49 | 0 |
| ATOM | 1311 | N | LEU | B2052 | 6.968 | 3.520 | 31.413 | 1.00 19.18 | N |
| MOTA | 1312 | CA | LEU | B2052 | 7.096 | 2.109 | 31.788 | 1.00 18.14 | C |
| MOTA | 1313 | CB | | B2052 | 5.782 | 1.616 | 32.419 | 1.00 18.69 | C |
| MOTA | 1314 | CG | | B2052 | 5.668 | 0.154 | 32.868 | 1.00 19.58 | C |
| MOTA | 1315 | CD1 | LEU | B2052 | 6.783 | -0.189 | 33.861 | 1.00 19.24 | C |
| ATOM | 1316 | CD2 | | B2052 | 4.299 | -0.070 | 33.511 | 1.00 20.41 | C |
| MOTA | 1317 | С | | B2052 | 7.476 | 1.209 | 30.598 | 1.00 17.54 | C |
| MOTA | 1318 | 0 | LEU | B2052 | 8.347 | 0.347 | 30.719 | 1.00 16.53 | 0 |
| ATOM | 1319 | N | ALA | B2053 | 6.828 | 1.411 | 29.453 | 1.00 16.29 | N |
| ATOM | 1320 | CA | | B2053 | 7.115 | 0.600 | 28.262 | 1.00 16.39 | С |
| MOTA | 1321 | CB | ALA | B2053 | 6.106 | 0.926 | 27.154 | 1.00 16.13 | C |
| ATOM | 1322 | С | ALA | B2053 | 8.550 | 0.794 | 27.744 | 1.00 15.79 | С |
| ATOM | 1323 | 0 | ALA | B2053 | 9.206 | -0.169 | 27.325 | 1.00 16.28 | 0 |
| ATOM | 1324 | N | GLY | B2054 | 9.034 | 2.033 | 27.771 | 1.00 15.48 | N |
| ATOM | 1325 | CA | | B2054 | 10.391 | 2.311 | 27.316 | 1.00 15.32 | С |
| MOTA | 1326 | С | | B2054 | 11.471 | 1.701 | 28.201 | 1.00 16.07 | C |
| ATOM | 1327 | 0 | | B2054 | 12.550 | 1.309 | 27.716 | 1.00 14.96 | 0 |
| ATOM | 1328 | N | | B2055 | 11.208 | 1.633 | 29.506 | 1.00 15.22 | N |
| ATOM | 1329 | CA | | B2055 | 12.179 | 1.040 | 30.430 | 1.00 16.35 | С |
| MOTA | 1330 | СВ | | B2055 | 11.790 | 1.353 | 31.886 | 1.00 17.42 | С |
| ATOM | 1331 | CG | | B2055 | 12.545 | 2.543 | 32.514 | 1.00 19.58 | С |
| | | | | | | | | | |

| ATOM | 1332 | CD | ARG | B2055 | 12.545 | 3.794 | 31.623 | 1.00 21.46 | С |
|------|------|-----|-----|---------|--------|---------|--------|--------------------------|---------------|
| ATOM | 1333 | NE | ARG | B2055 | 13.423 | 4.838 | 32.153 | 1.00 21.36 | - N |
| ATOM | 1334 | CZ | ARG | B2055 | 13.695 | 5.986 | 31.534 | 1.00 22.03 | С |
| MOTA | 1335 | NH1 | ARG | B2055 | 13.155 | 6.256 | 30.353 | 1.00 22.33 | N |
| ATOM | 1336 | NH2 | ARG | B2055 | 14.520 | 6.865 | 32.094 | 1.00 21.30 | N |
| MOTA | 1337 | С | ARG | B2055 | 12.261 | -0.479 | 30.194 | 1.00 16.15 | С |
| MOTA | 1338 | 0 | ARG | B2055 | 13.339 | -1.079 | 30.277 | 1.00 15.13 | 0 |
| ATOM | 1339 | N | TRP | B2056 | 11.119 | -1.090 | 29.884 | 1.00 16.30 | N |
| MOTA | 1340 | CA | TRP | B2056 | 11.055 | -2.528 | 29.608 | 1.00 17.26 | С |
| ATOM | 1341 | CB | TRP | B2056 | 9.592 | -2.966 | 29.425 | 1.00 19.31 | С |
| ATOM | 1342 | CG | TRP | B2056 | 9.393 | -4.449 | 29.444 | 1.00 22.46 | С |
| ATOM | 1343 | CD2 | TRP | B2056 | 9.458 | -5.335 | 28.325 | 1.00 24.24 | С |
| ATOM | 1344 | CE2 | TRP | B2056 | 9.234 | -6.644 | 28.813 | 1.00 25.47 | С |
| MOTA | 1345 | CE3 | TRP | B2056 | 9.684 | -5.153 | 26.954 | 1.00 25.79 | С |
| ATOM | 1346 | CD1 | TRP | B2056 | 9.139 | -5.234 | 30.540 | 1.00 23.87 | С |
| ATOM | 1347 | NE1 | TRP | B2056 | 9.041 | -6.552 | 30.167 | 1.00 24.64 | N |
| ATOM | 1348 | CZ2 | TRP | B2056 | 9.231 | -7.763 | 27.979 | 1.00 26.38 | С |
| ATOM | 1349 | CZ3 | TRP | B2056 | 9.681 | -6.270 | 26.122 | 1.00 27.06 | С |
| ATOM | 1350 | CH2 | TRP | B2056 | 9.455 | -7.559 | 26.641 | 1.00 27.05 | С |
| ATOM | 1351 | С | TRP | B2056 | 11.843 | -2.850 | 28.327 | 1.00 16.16 | С |
| ATOM | 1352 | 0 | TRP | B2056 | 12.642 | -3.794 | 28.288 | 1.00 16.26 | 0 |
| ATOM | 1353 | N | SER | B2057 | 11.608 | -2.053 | 27.288 | 1.00 15.01 | N |
| ATOM | 1354 | CA | | B2057 | 12.265 | -2.208 | 25.980 | 1.00 14.82 | С |
| ATOM | 1355 | CB | SER | B2057 | 11.678 | -1.155 | 25.017 | 1.00 15.72 | С |
| ATOM | 1356 | OG | SER | B2057 | 12.069 | -1.352 | 23.670 | 1.00 19.47 | 0 |
| MOTA | 1357 | С | SER | B2057 | 13.807 | -2.052 | 26.087 | 1.00 14.21 | С |
| ATOM | 1358 | 0 | SER | B2057 | 14.581 | -2.816 | 25.471 | 1.00 12.39 | 0 |
| ATOM | 1359 | N | ALA | B2058 | 14.246 | -1.072 | 26.873 | 1.00 12.21 | N |
| ATOM | 1360 | CA | ALA | B2058 | 15.680 | -0.810 | 27.052 | 1.00 12.92 | С |
| MOTA | 1361 | СВ | ALA | B2058 | 15.878 | 0.516 | 27.800 | 1.00 12.17 | С |
| ATOM | 1362 | С | ALA | B2058 | 16.398 | -1.949 | 27.801 | 1.00 12.59 | С |
| ATOM | 1363 | 0 | ALA | B2058 | 17.507 | -2.354 | 27.428 | 1.00 11.75 | 0 |
| ATOM | 1364 | N | LYS | B2059 | 15.772 | -2.455 | 28.861 | 1.00 12.47 | N |
| ATOM | 1365 | CA | LYS | B2059 | 16.368 | -3.546 | 29.634 | 1.00 13.35 | С |
| ATOM | 1366 | CB | LYS | B2059 | 15.579 | -3.757 | 30.947 | 1.00 14.19 | С |
| ATOM | 1367 | CG | LYS | B2059 | 15.656 | -2.538 | 31.896 | 1.00 14.71 | С |
| ATOM | 1368 | CD | LYS | B2059 | 14.961 | -2.754 | 33.258 | 1.00 15.04 | С |
| MOTA | 1369 | CE | LYS | B2059 | 15.045 | -1.488 | 34.124 | 1.00 16.38 | С |
| MOTA | 1370 | NZ | LYS | B2059 | 14.590 | -1.651 | 35.545 | 1.00 15.99 | N |
| MOTA | 1371 | С | LYS | B2059 | 16.459 | -4.846 | 28.814 | 1.00 14.13 | C |
| MOTA | 1372 | 0 | LYS | B2059 | 17.406 | -5.632 | 28.992 | 1.00 13.94 | 0 |
| ATOM | 1373 | N | GLU | B2060 | 15.500 | -5.072 | 27.907 | 1.00 13.55 | N |
| ATOM | 1374 | CA | GLU | B2060 | 15.535 | -6.276 | 27.066 | 1.00 14.73 | C |
| MOTA | 1375 | CB | GLU | B2060 | 14.160 | -6.552 | 26.436 | 1.00 16.24 | С |
| MOTA | 1376 | CG | | B2060 | 14.173 | -7.696 | 25.413 | 1.00 20.48 | C |
| ATOM | 1377 | CD | | J B2060 | 14.283 | -9.089 | 26.037 | 1.00 23.43 | C |
| ATOM | 1378 | | | J B2060 | 14.802 | | 27.168 | 1.00 26.30 | 0 |
| ATOM | 1379 | | | J B2060 | | -10.061 | 25.376 | 1.00 25.45 | O C |
| MOTA | 1380 | С | | B2060 | 16.608 | -6.174 | 25.960 | 1.00 13.95 | |
| MOTA | 1381 | 0 | | J B2060 | 17.238 | | 25.609 | 1.00 13.52 | O N |
| MOTA | 1382 | N | | B2061 | 16.819 | | 25.418 | 1.00 13.22 | и С |
| MOTA | 1383 | CA | | A B2061 | 17.838 | | 24.379 | 1.00 13.62 | c |
| MOTA | 1384 | CB | | A B2061 | 17.740 | | 23.801 | 1.00 13.16 1.00 13.67 | c |
| MOTA | 1385 | C | | A B2061 | 19.241 | | 24.950 | 1.00 13.67 | 0 |
| MOTA | 1386 | 0 | | A B2061 | 20.107 | | 24.257 | 1.00 14.02 | N |
| ATOM | 1387 | N | | E B2062 | 19.463 | | 26.207 | | C |
| MOTA | 1388 | CA | PHI | E B2062 | 20.760 | -4.860 | 26.873 | 1.00 14.50 | C |

| ATOM | 1389 | CB | PHE | B2062 | 20.844 | -4.049 | 28.185 | 1.00 14.44 | С |
|--------------|--------------|----------|-----|-------|--------|---------|--------|------------|-----|
| ATOM | 1390 | | | B2062 | 22.074 | -4.353 | 29.029 | 1.00 14.90 | С |
| ATOM | 1391 | CD1 | PHE | B2062 | 22.084 | -5.445 | 29.908 | 1.00 15.30 | С |
| ATOM | 1392 | | | B2062 | 23.223 | -3.571 | 28.923 | 1.00 15.56 | С |
| ATOM | 1393 | | | B2062 | 23.223 | -5.752 | 30.663 | 1.00 15.94 | С |
| ATOM | 1394 | | | B2062 | 24.375 | -3.869 | 29.678 | 1.00 15.34 | С |
| ATOM | 1395 | | | B2062 | 24.370 | -4.961 | 30.545 | 1.00 15.50 | С |
| MOTA | 1396 | | | B2062 | 20.969 | -6.363 | 27.147 | 1.00 14.72 | С |
| ATOM | 1397 | | | B2062 | 22.063 | -6.894 | 26.938 | 1.00 14.93 | 0 |
| ATOM | 1398 | | | B2063 | 19.922 | -7.052 | 27.599 | 1.00 14.63 | N |
| ATOM | 1399 | | | B2063 | 20.016 | -8.490 | 27.864 | 1.00 15.27 | С |
| ATOM | 1400 | CB | | B2063 | 18.688 | -9.021 | 28.415 | 1.00 16.20 | С |
| ATOM | 1401 | OG | | B2063 | 18.406 | -8.473 | 29.694 | 1.00 18.16 | 0 |
| ATOM | 1402 | C | | B2063 | 20.379 | -9.257 | 26.579 | 1.00 15.62 | С |
| ATOM | 1403 | 0 | | B2063 | | -10.185 | 26.607 | 1.00 14.45 | Ō |
| ATOM | 1404 | | | B2064 | 19.767 | -8.872 | 25.459 | 1.00 15.61 | N |
| ATOM | 1405 | | | B2064 | 20.049 | -9.514 | 24.175 | 1.00 16.52 | С |
| ATOM | 1406 | | | B2064 | 19.012 | -9.077 | 23.125 | 1.00 16.00 | c |
| ATOM | 1407 | CG | | B2064 | 17.614 | -9.664 | 23.369 | 1.00 15.31 | Ċ |
| ATOM | 1408 | CD | | B2064 | 16.563 | -9.149 | 22.365 | 1.00 17.09 | Ċ |
| ATOM | 1409 | CE | | B2064 | 16.849 | -9.635 | 20.935 | 1.00 18.35 | ċ |
| ATOM | 1410 | NZ | | B2064 | 15.798 | -9.213 | 19.951 | 1.00 19.10 | N |
| | | C | | B2064 | 21.470 | -9.195 | 23.694 | 1.00 17.20 | C |
| ATOM | 1411 | | | B2064 | | -10.024 | 23.043 | 1.00 17.20 | ō |
| ATOM | 1412 | 0 | | B2065 | 21.962 | -7.999 | 24.014 | 1.00 18.06 | N |
| ATOM | 1413 | N | | B2065 | 23.316 | -7.605 | 23.623 | 1.00 19.56 | C |
| ATOM | 1414 | CA CB | | B2065 | 23.545 | -6.119 | 23.922 | 1.00 20.35 | Č |
| ATOM | 1415 | СВ | | B2065 | 24.361 | -8.453 | 24.358 | 1.00 21.22 | Č |
| ATOM | 1416 | 0 | | B2065 | 25.473 | -8.657 | 23.859 | 1.00 20.91 | ō |
| ATOM | 1417 | | | B2065 | 24.007 | -8.940 | 25.545 | 1.00 22.79 | N |
| MOTA | 1418 | N | | B2066 | 24.924 | -9.774 | 26.331 | 1.00 25.40 | C |
| MOTA | 1419 | CA CB | | B2066 | 24.690 | -9.573 | 27.836 | 1.00 25.98 | Č |
| MOTA | 1420 1421 | CG | | B2066 | 25.035 | -8.178 | 28.353 | 1.00 28.04 | c |
| ATOM | | SD | | B2066 | 26.596 | -8.065 | 29.288 | 1.00 31.65 | S |
| ATOM | 1422 1423 | CE | | B2066 | 26.043 | -8.670 | 30.858 | 1.00 29.68 | Č |
| ATOM | | | | B2066 | | -11.256 | 25.983 | 1.00 26.28 | č |
| ATOM | 1424 1425 | C O | | B2066 | | -12.095 | 26.441 | 1.00 27.12 | Ō |
| ATOM | 1425 | N | | B2067 | | -11.570 | 25.184 | 1.00 26.98 | N |
| ATOM ATOM | 1427 | CA | | B2067 | | -12.943 | 24.772 | 1.00 28.85 | C |
| ATOM | 1428 | C | | B2067 | | -13.728 | 25.544 | 1.00 30.30 | Ċ |
| ATOM | 1429 | o | | B2067 | | -14.950 | 25.408 | 1.00 30.22 | 0 |
| MOTA | 1430 | N | | B2068 | | -13.048 | 26.335 | 1.00 31.36 | N |
| ATOM | 1431 | CA | | B2068 | | -13.729 | 27.120 | 1.00 33.00 | C |
| ATOM | 1431 | CB | | B2068 | | -13.892 | 28.595 | 1.00 32.89 | C |
| | 1432 | | | B2068 | | -14.628 | 29.332 | 1:00 33.56 | 0 |
| ATOM ATOM | 1433 | | | B2068 | | -12.528 | 29.248 | 1.00 32.58 | C |
| ATOM | 1435 | C | | B2068 | | -13.023 | 27.083 | 1.00 33.93 | C |
| ATOM | 1436 | Ö | | B2068 | | -12.381 | 26.091 | 1.00 34.69 | 0 |
| ATOM | 1437 | N | | B2069 | | -13.157 | 28.161 | 1.00 35.37 | . И |
| ATOM | 1438 | CA | | B2069 | | -12.534 | 28.239 | 1.00 36.59 | С |
| ATOM | 1439 | C | | B2069 | | -11.870 | 29.586 | 1.00 37.70 | C |
| ATOM | 1440 | 0 | | B2069 | | -12.221 | 30.580 | 1.00 38.22 | Ō |
| ATOM | 1441 | N | | B2000 | | -10.918 | 29.631 | 1.00 38.74 | N |
| ATOM | 1442 | CA | | B2070 | | -10.195 | 30.869 | 1.00 39.48 | C |
| ATOM | 1443 | CB | | B2070 | 14.789 | | 30.595 | 1.00 39.69 | Ċ |
| ATOM | 1444 | | | B2070 | 13.430 | | 30.057 | 1.00 40.00 | c |
| ATOM | 1445 | | | B2070 | 14.621 | | 31.880 | 1.00 39.65 | Ċ |
| 111011 | 1117 | 501 | | | 11.021 | | | | |

| ATOM | 1446 | CD1 | TLE | B2070 | 15.923 | -7.652 | 32.491 | 1.00 39.07 | С |
|------|------|-----|-----|---------|--------|---------|------------------|-------------|-----|
| ATOM | 1447 | | | B2070 | | -11.043 | 31.960 | 1.00 40.17 | С |
| ATOM | 1448 | | | B2070 | | -10.748 | 33.150 | 1.00 40.22 | 0 |
| ATOM | 1449 | | | B2071 | | -12.087 | 31.564 | 1.00 40.66 | N |
| ATOM | 1450 | | | B2071 | | -12.963 | 32.539 | 1.00 41.23 | C |
| | | | | B2071 | | -13.965 | 31.841 | 1.00 41.77 | Č |
| ATOM | 1451 | | | | | -13.319 | 31.185 | 1.00 43.00 | ő |
| ATOM | 1452 | | | B2071 | | -13.729 | 33.324 | 1.00 41.05 | č |
| ATOM | 1453 | | | B2071 | | -14.202 | 34.435 | 1.00 41.50 | 0 |
| ATOM | 1454 | | | B2071 | | | | 1.00 41.50 | N |
| ATOM | 1455 | | | B2072 | | -13.838 | 32.740 33.360 | 1.00 40.00 | C |
| ATOM | 1456 | | | B2072 | | -14.554 | | 1.00 40.65 | C |
| ATOM | 1457 | | | B2072 | | -15.336 | 32.286 | | C |
| ATOM | 1458 | | | B2072 | | -16.186 | 31.383 | 1.00 41.38 | |
| ATOM | 1459 | | | B2072 | | -16.871 | 30.301 | 1.00 42.22 | C |
| ATOM | 1460 | | | B2072 | | -17.749 | 29.419 | 1.00 42.85 | |
| ATOM | 1461 | | | B2072 | | -16.964 | 28.747 | 1.00 43.40 | Ń |
| ATOM | 1462 | | | B2072 | • | -13.620 | 34.093 | 1.00 38.99 | C |
| ATOM | 1463 | | | B2072 | | -13.947 | 35.174 | 1.00 38.73 | 0 |
| ATOM | 1464 | | | B2073 | | -12.457 | 33.502 | 1.00 38.00 | N |
| ATOM | 1465 | CA | LEU | B2073 | | -11.480 | 34.082 | 1.00 37.21 | С |
| ATOM | 1466 | CB | LEU | B2073 | 19.514 | -10.444 | 33.015 | 1.00 37.84 | С |
| MOTA | 1467 | | | B2073 | 20.842 | -9.689 | 33.144 | 1.00 38.45 | С |
| MOTA | 1468 | CD1 | LEU | B2073 | 21.202 | -9.069 | 31.801 | 1.00 38.77, | С |
| ATOM | 1469 | CD2 | LEU | B2073 | 20.738 | -8.625 | 34.226 | 1.00 38.87 | С |
| ATOM | 1470 | С | LEU | B2073 | 18.583 | -10.784 | 35.338 | 1.00 36.22 | С |
| ATOM | 1471 | 0 | LEU | B2073 | 19.335 | -10.491 | 36.268 | 1.00 36.38 | 0 |
| ATOM | 1472 | N | GLY | B2074 | 17.276 | -10.527 | 35.366 | 1.00 34.86 | N |
| ATOM | 1473 | CA | GLY | B2074 | 16.670 | -9.874 | 36.520 | 1.00 32.86 | C |
| ATOM | 1474 | С | GLY | B2074 | 16.457 | -8.376 | 36.351 | 1.00 31.51 | С |
| ATOM | 1475 | ō | | B2074 | 17.415 | -7.625 | 36.168 | 1.00 31.09 | 0 |
| ATOM | 1476 | N | | B2075 | 15.204 | | 36.435 | 1.00 29.86 | N |
| ATOM | 1477 | CA | | B2075 | 14.873 | -6.516 | 36.274 | 1.00 28.90 | С |
| MOTA | 1478 | CB | | B2075 | 13.348 | -6.309 | 36.264 | 1.00 29.85 | С |
| ATOM | 1479 | CG | | B2075 | 12.656 | -6.885 | 35.062 | | C |
| ATOM | 1480 | | | B2075 | 12.145 | -8.177 | 35.090 | 1.00 31.57 | С |
| ATOM | 1481 | | | B2075 | 12.502 | -6.130 | 33.905 | 1.00 31.69 | C |
| ATOM | 1482 | | | B2075 | 11.487 | -8.714 | 33.980 | 1.00 31.82 | С |
| ATOM | 1483 | | | B2075 | 11.845 | -6.656 | 32.786 | 1.00 32.40 | С |
| ATOM | 1484 | CZ | | B2075 | 11.336 | -7.954 | 32.828 | 1.00 32.18 | С |
| MOTA | 1485 | C | | B2075 | 15.470 | | 37.310 | 1.00 27.58 | С |
| ATOM | 1486 | Ö | | B2075 | 15.773 | | 36.983 | 1.00 26.85 | 0 |
| ATOM | 1487 | N | | B2076 | 15.626 | | 38.551 | 1.00 26.42 | N |
| MOTA | 1488 | CA | | B2076 | 16.161 | | 39.612 | 1.00 26.02 | C |
| MOTA | 1489 | CB | | B2076 | 15.829 | | 40.995 | 1.00 26.15 | Ċ |
| ATOM | 1490 | CG | | B2076 | 14.332 | -5.838 | 41.292 | 1.00 25.92 | C |
| ATOM | 1490 | | | B2076 | 13.641 | -4.482 | 41.284 | 1.00 26.13 | d |
| | 1491 | CD | | B2076 | 12.615 | | 40.624 | 1.00 25.80 | d |
| ATOM | | | | B2076 | 14.193 | | 42.031 | 1.00 25.89 | N |
| ATOM | 1493 | | | B2076 | 17.663 | | 39.524 | 1.00 25.52 | Ċ |
| MOTA | 1494 | С | | | 18.195 | | 40.276 | 1.00 25.32 | Č |
| MOTA | 1495 | 0 | | B2076 | | | 38.608 | 1.00 25.07 | N |
| ATOM | 1496 | N | | B2077 | 18.343 | | 38.448 | 1.00 25.24 | , C |
| ATOM | 1497 | CA | | B2077 | 19.789 | | | 1.00 23.24 | Č |
| ATOM | 1498 | CB | | B2077 | 20.447 | | 38.060 | 1.00 28.16 | C |
| ATOM | 1499 | CG | | P B2077 | 20.008 | | | 1.00 31.24 | |
| ATOM | 1500 | | | P B2077 | 19.868 | | 40.172 | | |
| ATOM | 1501 | | | P B2077 | 19.815 | | 38.407 | 1.00 34.01 | |
| ATOM | 1502 | C | ASE | P B2077 | 20.164 | -4.350 | 37.402 | 1.00 23.27 | C |

| MOTA | 1503 | 0 | ASP | B2077 | 21.347 | -4.096 | 37.173 | 1.00 2 | 3.32 | 0 | |
|------|------|-----|-------|---------|--------|-----------|--------|--------|-------|-----|-----|
| ATOM | 1504 | N | LEU | B2078 | 19.160 | -3.742 | 36.774 | 1.00 2 | 1.03 | N | |
| ATOM | 1505 | CA | | B2078 | 19.376 | -2.717 | 35.746 | 1.00 1 | 8.79 | C | |
| ATOM | 1506 | CB | | B2078 | 18.923 | -3.240 | 34.370 | 1.00 1 | 8.82 | C | |
| ATOM | 1507 | CG | | B2078 | 19.560 | | 33.861 | 1.00 1 | 9.30 | С | |
| ATOM | 1508 | | | B2078 | 18.877 | | 32.575 | 1.00.1 | 9.23 | С | |
| ATOM | 1509 | | | B2078 | 21.040 | | 33.622 | 1.00 1 | 9.43 | С | |
| ATOM | 1510 | C | | B2078 | 18.582 | | 36.081 | 1.00 1 | | С | |
| ATOM | 1511 | Ö | | B2078 | 17.463 | | 36.591 | 1.00 1 | | 0 | |
| ATOM | 1512 | N | | B2079 | 19.150 | | 35.792 | 1.00 1 | | N | |
| ATOM | 1513 | CA | | B2079 | 18.466 | | 36.060 | 1.00 1 | | С | |
| | 1514 | CB | | B2079 | 18.912 | | 37.417 | 1.00 1 | | C | |
| ATOM | 1514 | CG | | B2079 | 18.136 | | 37.863 | 1.00 1 | | C | |
| ATOM | 1516 | CD | | B2079 | 18.567 | | 39.237 | 1.00 1 | | C | |
| ATOM | | | | B2079 | 19.725 | | 39.376 | 1.00 1 | | 0 | |
| ATOM | 1517 | | | B2079 | 17.743 | | 40.180 | 1.00 2 | | C | |
| ATOM | 1518 | | | B2079 | 18.729 | | 34.944 | 1.00 | | C | |
| ATOM | 1519 | C | | | | | 34.543 | 1.00 | | Ċ | |
| MOTA | 1520 | 0 | | B2079 | 19.884 | | 34.452 | 1.00 | | N | |
| MOTA | 1521 | N | | B2080 | 17.659 | | 33.371 | 1.00 | | Ċ | |
| ATOM | 1522 | CA | | B2080 | 17.735 | | 32.083 | 1.00 | | ٠ ، | |
| MOTA | 1523 | CB | | B2080 | 16.973 | | 30.963 | 1.00 | | Č | |
| ATOM | 1524 | | | B2080 | 17.063 | | 31.593 | 1.00 | | Č | |
| MOTA | 1525 | | | B2080 | 17.55 | | | 1.00 | | | |
| ATOM | 1526 | С | | B2080 | 17.120 | | 33.779 | 1.00 | | Č | |
| MOTA | 1527 | 0 | | B2080 | 15.913 | | 34.046 | 1.00 | | 1 | |
| MOTA | 1528 | N | | B2081 | 17.94 | | 33.815 | | | | |
| ATOM | 1529 | CA | | B2081 | 17.46 | | 34.178 | 1.00 | | | |
| ATOM | 1530 | CB | | B2081 | 18.24 | | 35.398 | 1.00 | | | |
| ATOM | 1531 | CG | | B2081 | 18.45 | | 36.621 | 1.00 | | (| |
| MOTA | 1532 | | | B2081 | 19.40 | | 37.602 | 1.00 | | | |
| ATOM | 1533 | CD2 | | B2081 | 17.12 | | 37.296 | 1.00 | | (| |
| ATOM | 1534 | С | LEU | B2081 | 17.65 | | 33.006 | 1.00 | | | 2 |
| MOTA | 1535 | 0 | | B2081 | 18.25 | | 31.984 | 1.00 | | |) |
| MOTA | 1536 | N | | B2082 | 17.14 | | 33.159 | 1.00 | | | N - |
| MOTA | 1537 | CA | | B2082 | 17.27 | | 32.125 | 1.00 | | | 2 |
| ATOM | 1538 | CB | ASN | 1 B2082 | 15.89 | | 31.770 | 1.00 | | | 2 |
| MOTA | 1539 | CG | | 1 B2082 | 15.11 | | 30.816 | 1.00 | | | C |
| MOTA | 1540 | | | ₹ B2082 | 15.40 | | 29.619 | 1.00 | | | 0 |
| MOTA | 1541 | ND2 | ASN | N B2082 | 14.10 | | | 1.00 | | | N |
| MOTA | 1542 | С | | 1 B2082 | 18.17 | | 32.654 | | 23.63 | | C |
| ATOM | 1543 | 0 | | N B2082 | 17.98 | | | | 24.09 | | 0 |
| MOTA | 1544 | N | | N B2083 | 19.13 | | | | 24.20 | | N |
| MOTA | 1545 | CA | | N B2083 | 20.00 | | | | 25.17 | | C |
| MOTA | 1546 | CB | | N B2083 | 21.39 | | | | 25.74 | | C |
| MOTA | 1547 | CG | ASI | N B2083 | 21.40 | | | | 25.64 | | C |
| ATOM | 1548 | OD: | L ASI | N B2083 | 22.42 | | | | 27.52 | | 0 |
| MOTA | 1549 | ND2 | | N B2083 | 20.29 | | | | 24.85 | | N |
| MOTA | 1550 | С | AS | N B2083 | 19.35 | | | | 25.54 | | C |
| ATOM | 1551 | 0 | | N B2083 | 18.21 | | | | 25.60 | | 0 |
| MOTA | 1552 | N | | U B2084 | 20.06 | | | | 26.28 | | N |
| MOTA | 1553 | CA | _ | U B2084 | 19.49 | | | | 27.23 | | C |
| ATOM | 1554 | CB | | U B2084 | 20.37 | | | | 28.30 | | C |
| ATOM | 1555 | CG | GL | U B2084 | 21.73 | • | | | 29.51 | | C |
| ATOM | 1556 | CD | | U B2084 | 22.61 | | | | 31.00 | | C |
| MOTA | 1557 | OE | 1 GL | U B2084 | 22.06 | | | | 31.91 | | 0 |
| ATOM | 1558 | OE | | U B2084 | 23.84 | | | | 30.61 | | 0 |
| ATOM | 1559 | С | GL | U B2084 | 19.19 | 53 17.675 | 31.307 | 1.00 | 27.45 | | С |

| | | | | | | | 21 207 | 1.00 27.41 | 0 |
|------|------|-----|-----|---------|--------|--------|--------|-------------|--------|
| ATOM | 1560 | | | B2084 | 18.514 | | 31.207 | 1.00 27.41 | N |
| MOTA | 1561 | | | B2085 | 19.569 | | 30.244 | | C |
| MOTA | 1562 | | | B2085 | 19.259 | 17.429 | 28.885 | 1.00 27.29 | c |
| MOTA | 1563 | | | B2085 | 20.490 | | 27.976 | 1.00 29.07 | c |
| MOTA | 1564 | | | B2085 | 21.545 | | 28.244 | 1.00 30.86 | |
| MOTA | 1565 | CD | ARG | B2085 | 22.540 | 18.483 | 27.089 | 1.00 33.01 | C |
| MOTA | 1566 | NE | ARG | B2085 | 23.592 | 19.471 | 27.319 | 1.00 34.52 | N |
| ATOM | 1567 | | | B2085 | 24.556 | 19.337 | 28.221 | 1.00 34.97 | C |
| ATOM | 1568 | NH1 | ARG | B2085 | 24.608 | 18.252 | 28.982 | 1.00 36.01 | N |
| ATOM | 1569 | NH2 | ARG | B2085 | 25.469 | 20.285 | 28.363 | 1.00 35.52 | N |
| ATOM | 1570 | С | ARG | B2085 | 18.147 | 16.563 | 28.294 | 1.00 26.76 | С |
| ATOM | 1571 | 0 | ARG | B2085 | 17.642 | 16.838 | 27.203 | 1.00 26.29 | 0 |
| MOTA | 1572 | N | GLY | B2086 | 17.777 | 15.508 | 29.018 | 1.00 25.36 | N |
| MOTA | 1573 | CA | GLY | B2086 | 16.721 | 14.623 | 28.558 | 1.00 24.19 | С |
| ATOM | 1574 | С | | B2086 | 17.156 | 13.325 | 27.896 | 1.00 23.02 | С |
| ATOM | 1575 | Ö | | B2086 | 16.305 | 12.537 | 27.475 | 1.00 22.83 | 0 |
| ATOM | 1576 | N | | B2087 | 18.462 | 13.083 | 27.798 | 1.00 21.71 | N |
| MOTA | 1577 | CA | | B2087 | 18.938 | 11.848 | 27.172 | 1.00 20.63 | C |
| MOTA | 1578 | CB | | B2087 | 20.336 | 12.055 | 26.576 | 1.00 21.15 | C |
| ATOM | 1579 | C | | B2087 | 18.955 | 10.671 | 28.157 | 1.00 19.81 | С |
| ATOM | 1580 | Õ | | B2087 | 19.364 | 10.824 | 29.315 | 1.00 18.56 | 0 |
| ATOM | 1581 | N | | B2088 | 18.505 | 9.479 | 27.707 | 1.00 18.87 | N |
| ATOM | 1582 | CD | | B2088 | 17.864 | 9.249 | 26.397 | 1.00 19.36 | C |
| | | CA | | B2088 | 18.461 | 8.258 | 28.530 | 1.00 17.76 | С |
| ATOM | 1583 | | | B2088 | 17.442 | 7.390 | 27.790 | 1.00 18.59 | C |
| ATOM | 1584 | CB | | B2088 | 17.719 | 7.724 | 26.358 | 1.00 18.87 | С |
| ATOM | 1585 | CG | | | 19.831 | 7.571 | 28.650 | 1.00 16.87 | С |
| ATOM | 1586 | С | | B2088 | 20.593 | 7.559 | 27.688 | 1.00 15.25 | 0 |
| MOTA | 1587 | 0 | | B2088 | 20.130 | 7.002 | 29.826 | 1.00 16.14 | N |
| ATOM | 1588 | N | | B2089 | 21.405 | 6.311 | 30.078 | 1.00 16.26 | С |
| ATOM | 1589 | CA | | B2089 | 22.510 | 7.344 | 30.377 | 1.00 17.32 | Ċ |
| ATOM | 1590 | CB | | B2089 | 22.461 | 7.951 | 31.774 | 1.00 16.96 | ċ |
| ATOM | 1591 | CG | | B2089 | 23.255 | 7.445 | 32.810 | 1.00 18.32 | С |
| MOTA | 1592 | | | B2089 | 23.233 | 8.007 | 34.098 | 1.00 18.36 | C |
| MOTA | 1593 | | | B2089 | | 9.031 | 32.057 | 1.00 17.32 | С |
| MOTA | 1594 | CD2 | | B2089 | 21.625 | 9.595 | 33.332 | 1.00 18.67 | Č |
| MOTA | 1595 | CE2 | | B2089 | 21.580 | 9.079 | 34.347 | 1.00 18.08 | c |
| MOTA | 1596 | CZ | | B2089 | 22.379 | 9.654 | 35.601 | 1.00 19.43 | Ō |
| MOTA | 1597 | ОН | | B2089 | 22.337 | | 31.250 | 1.00 16.51 | c |
| ATOM | 1598 | С | | B2089 | 21.313 | 5.311 | 32.127 | 1.00 16.51 | Ö |
| MOTA | 1599 | 0 | | B2089 | 20.453 | 5.455 | 31.261 | 1.00 16.46 | N |
| MOTA | 1600 | N | | B2090 | 22.191 | 4.304 | | 1.00 16.71 | C |
| ATOM | 1601 | CA | | B2090 | 22.207 | 3.292 | 32.338 | 1.00 15.71 | Č |
| ATOM | 1602 | CB | | B2090 | 22.803 | 1.953 | 31.855 | 1.00 15.88 | Č |
| MOTA | 1603 | CG | | B2090 | 21.830 | 1.069 | 31.099 | 1.00 16.44 | Č |
| MOTA | 1604 | CD1 | PHE | B2090 | 21.652 | 1.216 | 29.724 | 1.00 16.46 | C |
| MOTA | 1605 | | | B2090 | 21.089 | 0.094 | 31.770 | | C |
| MOTA | 1606 | | | B2090 | 20.748 | 0.407 | 29.022 | 1.00 16.54 | C |
| MOTA | 1607 | | | E B2090 | 20.179 | | 31.084 | 1.00 16.80 | c |
| MOTA | 1608 | CZ | | E B2090 | 20.008 | -0.568 | 29.709 | 1.00 16.46 | C |
| MOTA | 1609 | С | | E B2090 | 23.027 | | 33.550 | 1.00 17.25. | |
| MOTA | 1610 | | | E B2090 | 24.245 | | 33.445 | | O N |
| MOTA | 1611 | N | SEI | R B2091 | 22.372 | | 34.700 | | N |
| MOTA | 1612 | CA | | R B2091 | 23.068 | | 35.922 | | C |
| ATOM | 1613 | CB | | R B2091 | 22.148 | | 36.802 | | С |
| MOTA | 1614 | OG | | R B2091 | 20.902 | | 37.052 | | 0 |
| ATOM | 1615 | | SE | R B2091 | 23.592 | | 36.729 | | C |
| ATOM | 1616 | 0 | SE | R B2091 | 24.479 | 3.255 | 37.582 | 1.00 18.83 | О |
| | | | | | | | | | |

| P | MOT | 1617 | N | GLN | B2092 | 23.048 | 1:920 | 36.448 | 1.00 | | N |
|---|--------------|--------------|---------|------|----------------|------------------|------------------|------------------|------|----------------|--------|
| 7 | MOT | 1618 | CA | GLN | B2092 | 23.438 | 0.675 | 37.116 | | 19.69 | С |
| P | MOTA | 1619 | CB | GLN | B2092 | 22.526 | 0.377 | 38.313 | | 21.62 | С |
| P | MOTA | 1620 | CG | | B2092 | 22.726 | 1.259 | 39.533 | | 25.05 | С |
| F | MOTA | 1621 | CD | | B2092 | 21.981 | 0.730 | 40.746 | | 27.87 | C |
| I | MOTA | 1622 | OE1 | GLN | B2092 | 20.775 | 0.944 | 40.900 | | 29.82 | 0 |
| Z | MOTA | 1623 | NE2 | | B2092 | 22.696 | 0.018 | 41.611 | | 29.02 | N |
| I | MOTA | 1624 | С | | B2092 | 23.336 | -0.512 | 36.151 | | 19.36 | C |
| 7 | MOTA | 1625 | 0 | | B2092 | 22.316 | -0.678 | 35.486 | | 18.36 | O M |
| 1 | MOTA | 1626 | N | | B2093 | 24.383 | -1.336 | 36.094 | | 18.90 | N C |
| 7 | MOTA | 1627 | CA | | B2093 | 24.411 | -2.514 | 35.221 | | 19.53 | C |
| 1 | MOTA | 1628 | CB | | B2093 | 24.441 | -2.073 | 33.755 | | 19.53 20.13 | C |
| | MOTA | 1629 | С | | B2093 | 25.625 | -3.407 | 35.524 36.024 | | 20.13 | Ö |
| | MOTA | 1630 | 0 | | B2093 | 26.641 | -2.928 | | | 21.00 | N |
| | MOTA | 1631 | N | | B2094 | 25.527 | -4.720 | 35.239 34.892 | | 21.48 | C |
| | MOTA | 1632 | CD | | B2094 | 24.303 | -5.472 | 35.498 | | 21.95 | č |
| | MOTA | 1633 | CA | | B2094 | 26.653 | -5.631 | 35.744 | | 22.34 | č |
| | MOTA | 1634 | CB | | B2094 | 25.956 | -6.963 | 34.739 | | 22.42 | c |
| | MOTA | 1635 | CG | | B2094 | 24.808 | -6.905 | 34.739 | | 22.30 | č |
| | MOTA | 1636 | С | | B2094 | 27.613 | -5.677 -6.690 | 33.594 | | 22.45 | ō |
| | ATOM | 1637 | 0 | | B2094 | 27.695 | -4.572 | 34.083 | | 22.56 | N |
| | ATOM | 1638 | N | | B2095 | 28.331 | -4.435 | 32.957 | | 23.11 | C |
| | ATOM | 1639 | CA | | B2095 | 29.267 28.471 | -4.433 | 31.688 | | 22.75 | Č |
| | ATOM | 1640 | CB | | B2095 | 29.307 | -3.979 | 30.439 | | 22.31 | Č |
| | ATOM | 1641 | CG | | B2095 | 29.484 | -2.746 | 29.812 | | 22.23 | C |
| | MOTA | 1642 | | | B2095 | 29.898 | -5.107 | 29.876 | | 22.30 | С |
| | ATOM | 1643 | | | B2095 B2095 | 30.237 | -2.639 | 28.640 | | 22.73 | С |
| | ATOM | 1644 | | | B2095 | 30.655 | -5.012 | 28.705 | | 22.36 | С |
| | ATOM | 1645 | | | B2095 | 30.825 | -3.774 | 28.085 | | 21.98 | C |
| | ATOM | 1646 | CZ C | | B2095 | 30.305 | -3.340 | 33.248 | | 23.62 | С |
| | ATOM | 1647 1648 | 0 | | B2095 | 29.965 | -2.284 | 33.778 | | 23.96 | 0 |
| | ATOM ATOM | 1649 | N | | B2096 | 31.561 | -3.584 | 32.884 | | 24.19 | N |
| | ATOM | 1650 | CA | | B2096 | 32.636 | -2.623 | 33.143 | 1.00 | 25.11 | С |
| | MOTA | 1651 | CB | | B2096 | 33.927 | -3.376 | 33.477 | | 26.30 | С |
| | ATOM | 1652 | OG | | B2096 | 33.722 | -4.306 | 34.523 | 1.00 | 28.33 | 0 |
| | ATOM | 1653 | c | | B2096 | 32.954 | -1.591 | 32.050 | 1.00 | 24.46 | С |
| | ATOM | 1654 | ō | | B2096 | 33.606 | -0.583 | 32.332 | 1.00 | 25.13 | 0 |
| | MOTA | 1655 | N | | B2097 | 32.513 | -1.828 | 30.818 | 1.00 | 23.39 | N |
| | ATOM | 1656 | CA | | B2097 | 32.818 | -0.891 | 29.739 | 1.00 | 21.60 | С |
| | ATOM | 1657 | C | | 82097 | 31.823 | 0.242 | 29.527 | | 20.27 | С |
| | MOTA | 1658 | ο. | GL) | 82097 | 31.138 | 0.651 | 30.460 | | 20.10 | 0 |
| | ATOM | 1659 | N | LYS | B2098 | 31.756 | 0.758 | 28.299 | | 19.44 | N |
| | ATOM | 1660 | CA | LYS | B2098 | 30.822 | 1.836 | 27.954 | | 17.90 | C |
| | ATOM | 1661 | CB | LYS | B2098 | 31.472 | 2.822 | | 1.00 | 20.19 | C |
| | MOTA | 1662 | CG | LYS | B2098 | 32.604 | 3.651 | 27.561 | | 21.96 | C |
| | MOTA | 1663 | CD | LYS | S B2098 | 33.055 | 4:682 | 26.543 | | 24.18 | С |
| | ATOM | 1664 | CE | LYS | S B2098 | 34.115 | 5.612 | 27.103 | | 25.70 | C |
| | MOTA | 1665 | NZ | | S B2098 | 34.538 | 6.626 | | | 27.22 | N |
| | MOTA | 1666 | С | | S B2098 | 29.561 | 1.256 | | | 16.51 | С |
| | MOTA | 1667 | | | S B2098 | 29.647 | 0.298 | | | 14.73 | O N |
| | MOTA | 1668 | | | E B2099 | 28.401 | | | | 15.59 | C |
| | ATOM | 1669 | | | E B2099 | 27.107 | | | | 15.02 | Ç |
| | MOTA | 1670 | | | E B2099 | 26.144 | | | | 0 15.10 | C |
| | MOTA | 1671 | | | E B2099 | 24.823 | | | | 0 16.11 | C |
| | ATOM | 1672 | | | E B2099 | 26.790 | | | | 0 15.18 | C |
| | MOTA | 1673 | CD | 1 IL | E B2099 | 25.994 | -0.462 | 30.363 | 1.0 | 0 16.41 | C |

| ATOM | 1674 | С | ILE | B2099 | 26.406 | 2.533 | 26.308 | 1.00 14.43 | С |
|------|------|-----|-----|---------|--------------------|---------------------|--------|------------|---|
| ATOM | 1675 | | ILE | B2099 | 26.039 | 3.551 | 26.900 | 1.00 14.51 | 0 |
| ATOM | 1676 | N | TRP | B2100 | 26.207 | 2.359 | 25.000 | 1.00 13.72 | N |
| ATOM | 1677 | CA | TRP | B2100 | 25.547 | 3.381 | 24.173 | 1.00 13.62 | С |
| ATOM | 1678 | | | B2100 | 26.342 | 3.558 | 22.864 | 1.00 13.58 | C |
| ATOM | 1679 | CG | | B2100 | 27.817 | 3.938 | 23.093 | 1.00 13.89 | C |
| ATOM | 1680 | | | B2100 | 28.334 | 5.257 | 23.347 | 1.00 13.95 | С |
| ATOM | 1681 | | | B2100 | 29.726 | 5.126 | 23.597 | 1.00 14.82 | С |
| ATOM | 1682 | | | B2100 | 27.755 | 6.535 | 23.395 | 1.00 14.46 | С |
| ATOM | 1683 | | | B2100 | 28.890 | 3.085 | 23.187 | 1.00 14.49 | С |
| ATOM | 1684 | | | B2100 | 30.041 | 3.795 | 23.492 | 1.00 14.89 | N |
| ATOM | 1685 | | | B2100 | 30.546 | 6.230 | 23.895 | 1.00 15.47 | С |
| ATOM | 1686 | | | B2100 | 28.577 | 7.640 | 23.697 | 1.00 15.28 | С |
| | 1687 | | | B2100 | 29.955 | 7.472 | 23.942 | 1.00 14.88 | С |
| ATOM | | C | | B2100 | 24.071 | 2.998 | 23.886 | 1.00 13.84 | С |
| MOTA | 1688 | | | B2100 | 23.816 | 1.995 | 23.214 | 1.00 13.89 | Ō |
| ATOM | 1689 | 0 | | B2100 | 23.120 | 3.808 | 24.379 | 1.00 13.08 | N |
| ATOM | 1690 | N | | | 21.657 | 3.557 | 24.239 | 1.00 12.41 | Ċ |
| ATOM | 1691 | CA | | B2101 | 21.059 | 3.267 | 25.634 | 1.00 13.29 | C |
| ATOM | 1692 | CB | | B2101 | | 3.353 | 25.825 | 1.00 13.23 | č |
| ATOM | 1693 | CG | | B2101 | 19.524 | | 25.355 | 1.00 12.28 | č |
| ATOM | 1694 | | | B2101 | 18.889 | 2.043 | 27.303 | 1.00 12.20 | c |
| MOTA | 1695 | | | B2101 | 19.156 | 3.601 4.674 | | 1.00 12.42 | C |
| MOTA | 1696 | C | | B2101 | 20.796 | | 23.602 | 1.00 11.61 | 0 |
| ATOM | 1697 | 0 | | B2101 | 21.063 | 5.858 | 23.811 | 1.00 11.01 | Ŋ |
| ATOM | 1698 | N | | B2102 | 19.760 | 4.287 | 22.844 | | C |
| MOTA | 1699 | CA | | B2102 | 18.799 | 5.237 | 22.237 | 1.00 11.37 | C |
| MOTA | 1700 | CB | | B2102 | 19.212 | 5.616 | 20.810 | 1.00 11.79 | |
| ATOM | 1701 | OG | | B2102 | 18.405 | 6.679 | 20.308 | 1.00 9.95 | 0 |
| MOTA | 1702 | С | | B2102 | 17.371 | 4.634 | 22.219 | 1.00 11.48 | С |
| MOTA | 1703 | 0 | | B2102 | 17.220 | 3.421 | 22.026 | 1.00 11.63 | 0 |
| MOTA | 1704 | N | | B2103 | 16.351 | 5.482 | 22.425 | 1.00 10.47 | N |
| MOTA | 1705 | CA | | B2103 | 14.912 | 5.096 | 22.465 | 1.00 10.97 | C |
| MOTA | 1706 | CB | | B2103 | 14.337 | 5.250 | 23.934 | 1.00 11.04 | C |
| MOTA | 1707 | | | B2103 | 12.852 | 4.835 | 23.981 | 1.00 11.15 | С |
| ATOM | 1708 | CG1 | ILE | B2103 | 15.136 | 4.390 | 24.924 | 1.00 10.41 | С |
| ATOM | 1709 | CD1 | | B2103 | 14.781 - | 4.658 | 26.424 | 1.00 10.59 | C |
| ATOM | 1710 | С | ILE | : B2103 | 14.042 | 5.995 | 21.536 | 1.00 11.56 | С |
| MOTA | 1711 | 0 | | B2103 | . 14.327 | 7.184 | 21.393 | 1.00 11.36 | 0 |
| MOTA | 1712 | N | SER | B2104 | 12.994 | 5.435 | 20.915 | 1.00 13.13 | N |
| MOTA | 1713 | CA | SER | R B2104 | 12.073 | 6.214 | 20.054 | 1.00 14.88 | C |
| MOTA | 1714 | CB | | R B2104 | 12.582 | 6.263 | 18.603 | 1.00 15.92 | C |
| ATOM | 1715 | OG | SEF | R B2104 | 11.787 | 7.132 | 17.789 | 1.00 16.21 | 0 |
| ATOM | 1716 | С | SEF | R B2104 | 10.652 | 5.617 | 20.070 | 1.00 15.87 | C |
| ATOM | 1717 | 0 | SEF | R B2104 | 10.485 | 4.418 | 20.297 | 1.00 15.32 | 0 |
| ATOM | 1718 | N | HIS | B2105 | [.] 9.623 | 6.429 | 19.822 | 1.00 17.79 | N |
| ATOM | 1719 | CA | HIS | B2105 | 8.266 | 5.872 | 19.833 | 1.00 19.31 | C |
| ATOM | 1720 | CB | HIS | B2105 | 7.683 | 5. -9 21 | 21.249 | 1.00 21.32 | C |
| MOTA | 1721 | CG | HIS | B2105 | 7.405 | 7.306 | 21.746 | 1.00 23.02 | C |
| MOTA | 1722 | CD2 | HIS | B2105 | 6.279 | 8.058 | 21.704 | 1.00 25.09 | С |
| MOTA | 1723 | ND1 | HIS | B2105 | 8.363 | 8.086 | 22.356 | 1.00 25.22 | N |
| ATOM | 1724 | CE1 | HIS | S B2105 | 7.841 | 9.260 | 22.669 | 1.00 25.65 | С |
| MOTA | 1725 | NE2 | HIS | B2105 | 6.577 | 9.269 | 22.285 | 1.00 26.41 | N |
| ATOM | 1726 | С | HIS | S B2105 | 7.237 | 6.486 | 18.870 | 1.00 20.14 | c |
| ATOM | 1727 | 0 | HIS | S B2105 | 7.453 | 7.560 | 18.305 | 1.00 18.58 | 0 |
| ATOM | 1728 | N | THE | R B2106 | 6.128 | 5.763 | 18.687 | 1.00 20.92 | N |
| ATOM | 1729 | | TH! | R B2106 | 5.008 | 6.208 | 17.852 | | C |
| ATOM | 1730 | | | R B2106 | 4.758 | 5.302 | 16.612 | 1.00 23.62 | С |
| | | | | | | | | | |

| ATOM | 1731 | OG1 | THR | B2106 | 4.237 | 4.035 | 17.039 | 1.00 24.37 | 0 |
|------|-------|-----|-----|---------|--------|--------|--------|------------|-----|
| ATOM | 1732 | | | B2106 | 6.043 | 5.092 | 15.820 | 1.00 23.72 | С |
| ATOM | 1733 | | | B2106 | 3.766 | 6.106 | 18.735 | 1.00 23.79 | С |
| ATOM | 1734 | | | B2106 | 3.867 | 5.875 | 19.937 | 1.00 24.63 | 0 |
| ATOM | 1735 | | | B2107 | 2.591 | 6.255 | 18.138 | 1.00 24.86 | N |
| | 1736 | | | B2107 | 1.355 | 6.176 | 18.906 | 1.00 24.83 | С |
| ATOM | | | | B2107 | 0.189 | 6.691 | 18.059 | 0.05 24.72 | Č |
| ATOM | 1737 | | | | -0.652 | 7.716 | 18.790 | 0.05 24.62 | Ċ |
| ATOM | 1738 | | | B2107 | | 7.710 | 19.844 | 0.05 24.64 | Ö |
| ATOM | 1739 | | | B2107 | -1.227 | | 18.312 | 0.05 24.51 | 0 |
| MOTA | 1740 | | | B2107 | -0.738 | 8.867 | | 1.00 24.92 | C |
| MOTA | 1741 | | | B2107 | 1.043 | 4.763 | 19.403 | | 0 |
| MOTA | 1742 | 0 | | B2107 | 0.368 | 4.598 | 20.421 | 1.00 26.07 | |
| ATOM | 1743 | N | | B2108 | 1.535 | 3.745 | 18.701 | 1.00 24.68 | N |
| ATOM | 1744 | CA | GLN | B2108 | 1.255 | 2.361 | 19.086 | 1.00 24.22 | C |
| MOTA | 1745 | CB | | B2108 | 0.522 | 1.652 | 17.939 | 1.00 25.96 | C |
| ATOM | 1746 | CG | GLN | B2108 | -0.753 | 2.352 | 17.462 | 1.00 27.90 | C |
| ATOM | 1747 | CD | GLN | B2108 | -1.328 | 1.732 | 16.189 | 1.00 29.69 | C |
| MOTA | 1748 | OE1 | GLN | B2108 | -2.371 | 1.073 | 16.215 | 1.00 31.19 | 0 |
| ATOM | 1749 | NE2 | GLN | B2108 | -0.641 | 1.940 | 15.069 | 1.00 30.55 | N |
| ATOM | 1750 | С | GLN | B2108 | 2.450 | 1.489 | 19.517 | 1.00 23.66 | С |
| MOTA | 1751 | 0 | GLN | B2108 | 2.246 | 0.490 | 20.216 | 1.00 22.94 | 0 |
| MOTA | 1752 | N | PHE | B2109 | 3.672 | 1.854 | 19.115 | 1.00 22.58 | N |
| ATOM | 1753 | CA | | B2109 | 4.869 | 1.058 | 19.450 | 1.00 22.19 | С |
| ATOM | 1754 | CB | | B2109 | 5.440 | 0.378 | 18.187 | 1.00 23.42 | C |
| ATOM | 1755 | CG | | B2109 | 4.409 | -0.256 | 17.287 | 1.00 25.28 | С |
| ATOM | 1756 | | | B2109 | 3.830 | 0.469 | 16.248 | 1.00 26.47 | С |
| ATOM | 1757 | | | B2109 | 4.038 | -1.586 | 17.459 | 1.00 26.35 | С |
| ATOM | 1758 | | | B2109 | 2.894 | -0.123 | 15.386 | 1.00 26.84 | С |
| | 1759 | | | B2109 | 3.106 | -2.190 | 16.607 | 1.00 27.41 | С |
| ATOM | 1760 | CZ | | B2109 | 2.534 | -1.454 | 15.567 | 1.00 27.07 | С |
| ATOM | | | | B2109 | 6.031 | 1.852 | 20.088 | 1.00 20.94 | С |
| ATOM | 1761 | C | | B2109 | 6.034 | 3.082 | 20.086 | 1.00 20.73 | 0 |
| ATOM | 1762 | 0 | | | 7.020 | 1.128 | 20.619 | 1.00 20.20 | N |
| ATOM | 1763 | N | | B2110 | 8.225 | 1.737 | 21.210 | 1.00 18.93 | C |
| ATOM | 1764 | CA | | B2110 | 8.115 | 1.867 | 22.761 | 1.00 19.35 | č |
| ATOM | 1765 | CB | | B2110 | | 0.496 | 23.404 | 1.00 13.33 | Ċ |
| MOTA | 1766 | | | B2110 | 7.968 | | 23.404 | 1.00 21.12 | c |
| ATOM | 1767 | | | B2110 | 9.339 | 2.595 | | 1.00 18.01 | c |
| ATOM | 1768 | С | | B2110 | 9.423 | 0.846 | 20.845 | 1.00 18.01 | o |
| MOTA | 1769 | 0 | | B2110 | 9.295 | -0.380 | 20.827 | 1.00 17.84 | N |
| MOTA | 1770 | N | | B2111 | 10.576 | 1.450 | 20.548 | 1.00 15.96 | C |
| MOTA | 1771 | CA | | B2111 | 11.768 | 0.678 | 20.170 | | C |
| MOTA | 1772 | CB | | B2111 | 11.950 | 0.693 | 18.628 | 1.00 17.10 | 0 |
| MOTA | 1773 | | | B2111 | 13.011 | -0.201 | 18.258 | 1.00 21.79 | C |
| MOTA | 1774 | | | B2111 | 12.283 | 2.096 | 18.141 | 1.00 17.28 | c |
| MOTA | 1775 | С | | B2111 | 13.049 | 1.203 | 20.839 | 1.00 14.55 | |
| MOTA | 1776 | 0 | | R B2111 | 13.122 | 2.380 | 21.194 | 1.00 12.59 | 0 |
| MOTA | 1777 | N | | B2112 | 14.044 | 0.326 | 21.005 | 1.00 13.42 | N |
| ATOM | 1.778 | CA | ALF | B2112 | 15.325 | | 21.644 | 1.00 12.71 | C |
| MOTA | 1779 | CB | | B2112 | 15.247 | | 23.145 | 1.00 12.85 | . с |
| MOTA | 1780 | C | | B2112 | 16.516 | | 21.024 | 1.00 12.80 | С |
| ATOM | 1781 | 0 | | A B2112 | 16.348 | | 20.535 | 1.00 13.45 | 0 |
| MOTA | 1782 | N | SEF | R B2113 | 17.709 | | 21.060 | 1.00 12.54 | N |
| ATOM | 1783 | CA | SEI | R B2113 | 18.937 | | 20.498 | 1.00 12.67 | C |
| ATOM | 1784 | CB | SEI | R B2113 | 19.222 | 0.539 | 19.115 | 1.00 12.72 | С |
| ATOM | 1785 | | | R B2113 | 20.402 | | 18.523 | 1.00 13.88 | 0 |
| ATOM | 1786 | | | R B2113 | 20.152 | | 21.443 | 1.00 11.86 | С |
| ATOM | 1787 | | | R B2113 | 20.326 | 1.247 | 21.973 | 1.00 12.14 | 0 |

| MOTA | 1788 | N | VAL | B2114 | 20.967 | -0.905 | 21.636 | 1.00 10.76 | N |
|------|------|------|-----|---------|--------|--------|--------|-------------|---|
| ATOM | 1789 | CA | VAL | B2114 | 22.157 | -0.885 | 22.526 | 1.00 11.02 | С |
| ATOM | 1790 | CB | VAL | B2114 | 21.912 | -1.748 | 23.810 | 1.00 10.07 | C |
| ATOM | 1791 | CG1 | VAL | B2114 | 23.204 | -1.874 | 24.619 | 1.00 12.63 | C |
| ATOM | 1792 | CG2 | VAL | B2114 | 20.808 | -1.124 | 24.689 | 1.00 11.23 | С |
| ATOM | 1793 | С | VAL | B2114 | 23.451 | -1.438 | 21.880 | 1.00 11.08 | С |
| ATOM | 1794 | 0 | VAL | B2114 | 23.408 | -2.477 | 21.204 | 1.00 10.49 | 0 |
| ATOM | 1795 | N | ILE | B2115 | 24.584 | -0.753 | 22.093 | 1.00 11.85 | N |
| ATOM | 1796 | CA | ILE | B2115 | 25.905 | -1.198 | 21.585 | 1.00 11.88 | C |
| ATOM | 1797 | CB | ILE | B2115 | 26.485 | -0.236 | 20.492 | 1.00 12.44 | С |
| ATOM | 1798 | CG2 | ILE | B2115 | 27.841 | -0.756 | 19.999 | 1.00 12.78 | С |
| ATOM | 1799 | CG1 | ILE | B2115 | 25.529 | -0.134 | 19.300 | 1.00 12.56 | С |
| ATOM | 1800 | CD1 | ILE | B2115 | 25.889 | 0.986 | 18.331 | 1.00 12.68 | С |
| ATOM | 1801 | С | ILE | B2115 | 26.883 | -1.197 | 22.782 | 1.00 12.95 | C |
| ATOM | 1802 | 0 | | B2115 | 26.966 | -0.197 | 23.507 | 1.00 13.03 | 0 |
| ATOM | 1803 | N | | B2116 | 27.600 | -2.306 | 22.994 | 1.00 12.77 | N |
| ATOM | 1804 | CA | | B2116 | 28.559 | -2.432 | 24.115 | 1.00 14.04 | C |
| ATOM | 1805 | СВ | | B2116 | 28.353 | -3.785 | 24.830 | 1.00 13.62 | С |
| ATOM | 1806 | CG | | B2116 | 26.929 | -4.093 | 25.349 | 1.00 14.05 | С |
| ATOM | 1807 | | | B2116 | 26.866 | -5.489 | 25.971 | 1.00 15.37 | С |
| ATOM | 1808 | | | B2116 | 26.520 | -3.055 | 26.384 | 1.00 14.15 | С |
| ATOM | 1809 | C | | B2116 | 30.020 | -2.296 | 23.630 | 1.00.14.81 | С |
| ATOM | 1810 | Ŏ | | B2116 | 30.381 | -2.839 | 22.582 | 1.00 14.52 | 0 |
| ATOM | 1811 | N | | B2117 | 30.858 | -1.605 | 24.409 | 1.00 16.40 | N |
| ATOM | 1812 | CA | | B2117 | 32.255 | -1.353 | 24.027 | 1.00 18.58 | С |
| ATOM | 1813 | CB | | B2117 | 32.344 | 0.062 | 23.426 | 1.00 18.84 | С |
| ATOM | 1814 | CG | | B2117 | 33.737 | 0.570 | 23.061 | 1.00 21.74 | С |
| ATOM | 1815 | CD | | B2117 | 33.703 | | 22.450 | 1.00 23.34 | C |
| ATOM | 1816 | | | B2117 | 33.161 | 2.908 | 23.098 | 1.00 22.55 | 0 |
| ATOM | 1817 | | | B2117 | 34.221 | 2.153 | 21.322 | 1.00 24.09 | 0 |
| ATOM | 1818 | C | | B2117 | 33.247 | -1.495 | 25.196 | 1.00 20.32 | С |
| ATOM | 1819 | Ö | | B2117 | 32.989 | -1.010 | 26.303 | 1.00 18.78 | 0 |
| ATOM | 1820 | И | | B2118 | 34.384 | -2.141 | 24.931 | 1.00 22.46 | N |
| ATOM | 1821 | CA | | B2118 | 35.413 | -2.366 | 25.949 | 1.00 26.31 | С |
| ATOM | 1822 | CB | | B2118 | 35.364 | -3.830 | 26.415 | 1.00 28.48 | С |
| ATOM | 1823 | CG | | B2118 | 36.185 | -4.151 | 27.657 | 1.00 31.58 | С |
| ATOM | 1824 | CD | | B2118 | 35.479 | -3.793 | 28.952 | 1.00 33.18 | С |
| MOTA | 1825 | | | B2118 | 34.479 | -4.464 | 29.295 | 1.00 34.62 | 0 |
| ATOM | 1826 | | | B2118 | 35.925 | -2.839 | 29.628 | 1.00 3,4.75 | 0 |
| ATOM | 1827 | C | | B2118 | 36.820 | -2.039 | 25.435 | 1.00 27.70 | С |
| ATOM | 1828 | o | | B2118 | 36.958 | -1.559 | 24.285 | 1.00 28.17 | 0 |
| ATOM | 1829 | | | B2118 | 37.784 | -2.267 | 26.199 | 1.00 29.81 | 0 |
| TER | 1830 | 0111 | | B2118 | | | | | |
| ATOM | 1831 | CB | | C3003 | 38.407 | 0.566 | 12.507 | 1.00 29.11 | С |
| ATOM | 1832 | CG | | C3003 | | -0.372 | | 1.00 32.10 | С |
| ATOM | 1833 | SD | | C3003 | 39.971 | 0.467 | 10.186 | 1.00 36.76 | S |
| ATOM | 1834 | CE | | C3003 | 41.535 | 0.656 | 11.078 | 1.00 35.20 | С |
| ATOM | 1835 | C | | C3003 | 36.229 | -0.625 | 12.723 | 1.00 24.49 | С |
| ATOM | 1836 | õ | | C3003 | 36.251 | -1.743 | 12.216 | 1.00 24.23 | 0 |
| ATOM | 1837 | N | | C3003 | 38.104 | -1.203 | 14.236 | 1.00 26.20 | N |
| ATOM | 1838 | CA | | C3003 | 37.432 | -0.097 | 13.493 | 1.00 26.22 | C |
| ATOM | 1839 | Ŋ | | C3003 | 35.182 | 0.190 | 12.648 | 1.00 22.87 | N |
| ATOM | 1840 | CA | | E C3004 | 33.960 | -0.165 | 11.933 | 1.00 21.52 | C |
| ATOM | 1841 | CB | | E C3004 | 32.800 | 0.781 | 12.355 | 1.00 21.32 | С |
| MOTA | 1842 | | | E C3004 | 31.535 | 0.469 | 11.557 | 1.00 21.05 | С |
| ATOM | 1843 | | | E C3004 | 32.547 | | 13.864 | 1.00 20.83 | Ċ |
| ATOM | 1844 | | | E C3004 | 31.537 | | 14.443 | | С |
| UION | 1011 | | | _ 05004 | 52.55 | | | | |

| ATOM | 1845 | С | ILE | C3004 | | 34.199 | -0.043 | 10.422 | 1.00 | | С |
|------|------|------|---------------------|---------|---|--------|--------|--------|------|-------|---|
| ATOM | 1846 | 0 | ILE | C3004 | | 34.938 | 0.848 | 9.979 | 1.00 | | 0 |
| MOTA | 1847 | N | VAL | C3005 | | 33.610 | -0.952 | 9.638 | 1.00 | | N |
| ATOM | 1848 | CA | VAL | C3005 | | 33.749 | -0.906 | 8.182 | 1.00 | | C |
| ATOM | 1849 | CB | VAL | C3005 | | 34.642 | -2.068 | 7.628 | 1.00 | | C |
| ATOM | 1850 | CG1 | VAL | C3005 | | 36.083 | -1.890 | 8.090 | 1.00 | | С |
| ATOM | 1851 | | | C3005 | | 34.109 | -3.413 | 8.076 | 1.00 | | С |
| ATOM | 1852 | С | | C3005 | | 32.413 | -0.901 | 7.422 | | 19.52 | С |
| ATOM | 1853 | 0 | | C3005 | | 32.411 | -0.880 | 6.192 | 1.00 | 19.11 | 0 |
| ATOM | 1854 | N | GLY | C3006 | | 31.289 | -0.906 | 8.149 | | 18.23 | N |
| ATOM | 1855 | CA | GLY | C3006 | | 29.974 | -0.880 | 7.508 | 1.00 | 17.17 | С |
| ATOM | 1856 | С | | C3006 | | 28.797 | -0.986 | 8.482 | | 16.61 | С |
| ATOM | 1857 | Ō | | C3006 | | 28.963 | -1.526 | 9.579 | | 16.76 | 0 |
| ATOM | 1858 | N | | C3007 | | 27.620 | -0.477 | 8.093 | 1.00 | 15.51 | N |
| ATOM | 1859 | CA | | C3007 | | 26.400 | -0.531 | 8.935 | 1.00 | 15.40 | С |
| ATOM | 1860 | СВ | | C3007 | | 26.418 | 0.624 | 9.953 | 1.00 | 15.15 | С |
| ATOM | 1861 | CG | | C3007 | | 25.191 | 0.709 | 10.821 | 1.00 | 14.61 | С |
| ATOM | 1862 | | | C3007 | | 24.430 | 1.772 | 11.180 | 1.00 | 14.84 | С |
| ATOM | 1863 | | | C3007 | | 24.668 | -0.377 | 11.493 | 1.00 | 15.01 | N |
| ATOM | 1864 | | | C3007 | | 23.639 | 0.013 | 12.229 | 1.00 | 15.56 | С |
| ATOM | 1865 | | | C3007 | | 23.475 | 1.313 | 12.058 | 1.00 | 15.15 | N |
| ATOM | 1866 | C | | C3007 | | 25.086 | -0.476 | 8.115 | 1.00 | 14.78 | С |
| MOTA | 1867 | Ö | | C3007 | | 24.933 | 0.372 | 7.228 | 1.00 | 14.49 | 0 |
| ATOM | 1868 | N | | C3008 | | 24.145 | -1.376 | 8.418 | 1.00 | 14.82 | N |
| ATOM | 1869 | CA | | C3008 | | 22.867 | -1.390 | 7.709 | 1.00 | 14.90 | С |
| MOTA | 1870 | C | | C3008 | | 21.668 | -1.918 | 8.495 | 1.00 | 15.74 | С |
| ATOM | 1871 | Ö | | C3008 | | 21.835 | -2.757 | 9.391 | 1.00 | 14.75 | 0 |
| MOTA | 1872 | N | | C3009 | | 20.465 | -1.425 | 8.166 | 1.00 | 15.25 | N |
| ATOM | 1873 | CA | | C3009 | | 19.211 | -1.847 | 8.823 | 1.00 | 15.66 | С |
| MOTA | 1874 | CB | | C3009 | | 18.692 | -0.769 | 9.837 | 1.00 | 14.95 | C |
| MOTA | 1875 | | | C3009 | | 19.789 | -0.421 | 10.873 | 1.00 | 15.05 | С |
| ATOM | 1876 | | | C3009 | | 18.261 | 0.492 | 9.079 | 1.00 | 14.33 | С |
| ATOM | 1877 | | | C3009 | | 17.632 | 1.555 | 9.956 | 1.00 | 14.63 | С |
| MOTA | 1878 | c | | C3009 | • | 18.090 | -2.102 | 7.780 | 1.00 | 16.20 | С |
| ATOM | 1879 | Õ | | C3009 | | 18.221 | -1.696 | 6.619 | 1.00 | 16.14 | 0 |
| ATOM | 1880 | N | | C3010 | | 17.004 | -2.762 | 8.204 | 1.00 | 16.80 | N |
| ATOM | 1881 | CA | | C3010 | | 15.853 | -3.080 | 7.330 | 1.00 | 17.32 | С |
| ATOM | 1882 | CB | | C3010 | | 16.130 | -4.365 | 6.527 | 1.00 | 18.68 | С |
| ATOM | 1883 | CG | | C3010 | | 14.977 | -4.741 | 5.579 | 1.00 | 18.99 | С |
| ATOM | 1884 | | | C3010 | | 14.852 | -4.105 | 4.518 | | 19.45 | 0 |
| ATOM | 1885 | | | C3010 | | 14.193 | -5.667 | 5.896 | | 19.42 | 0 |
| ATOM | 1886 | С | | P C3010 | | 14.549 | -3.290 | 8.120 | | 18.11 | С |
| ATOM | 1887 | | AS | P C3010 | | 14.580 | -3.711 | 9.283 | | 17.23 | 0 |
| ATOM | 1888 | N | IL | E C3011 | | 13.411 | -2.978 | 7.488 | | 17.97 | N |
| | 1889 | CA | IL | E C3011 | | 12.082 | -3.191 | 8.081 | | 18.54 | С |
| ATOM | 1890 | | | E C3011 | | 11.444 | -1.876 | 8.656 | | 18.66 | C |
| MOTA | 1891 | | | E C3011 | | 11.363 | -0.776 | 7.579 | | 19.04 | С |
| MOTA | 1892 | | | E C3011 | | 10.048 | -2.185 | | | 19.19 | С |
| MOTA | 1893 | | 1 IL | E C3011 | | 9.421 | -1.049 | | | 19.08 | С |
| ATOM | 1894 | | IL | E C3011 | | 11.207 | | | | 18.75 | С |
| ATOM | 1895 | | IL | E C3011 | | 11.286 | | | | 18.39 | 0 |
| ATOM | 1896 | | GL | U C3012 | | 10.389 | | | | 19.66 | N |
| ATOM | 1897 | | GL | U C3012 | | 9.544 | | | | 20.80 | C |
| MOTA | 1898 | СВ | GL | U C3012 | | 10.290 | | | | 22.15 | C |
| ATOM | 1899 | | GL | U C3012 | | 9.468 | | | | 23.49 | C |
| MOTA | 1900 | | | U C3012 | | 9.692 | | | | 24.70 | C |
| MOTA | 1901 | . OE | 1 GL | U C3012 | | 10.294 | -6.228 | 2.973 | 1.00 | 24.77 | 0 |
| | | | | | | | | | | | |

| ATOM | 1902 | OE2 | GLU (| C3012 | 9.258 | -8.095 | 2.460 | 1.00 25.5 | 0 | 0 |
|------|--------------|-----|-------|---------|-------|------------|--------|-----------|-----|---|
| ATOM | 1903 | С | GLU (| C3012 | 8.160 | -5.870 | 6.759 | 1.00 21.3 | | С |
| ATOM | 1904 | | GLU | C3012 | 8.049 | -6.431 | 7.848 | 1.00 20.3 | | 0 |
| ATOM | 1905 | | | C3013 | 7.111 | -5.614 | 5.971 | 1.00 22.0 | | N |
| ATOM | 1906 | | | C3013 | 5.743 | -6.004 | 6.345 | 1.00 23.4 | 3 | С |
| ATOM | 1907 | CB | | C3013 | 4.703 | | 5.534 | 1.00 24.6 | 0 | C |
| ATOM | 1908 | | | C3013 | 4.706 | | 5.716 | 1.00 26.5 | 2 . | C |
| | 1909 | CD | | C3013 · | 4.063 | | 7.018 | 1.00 28.4 | | С |
| ATOM | | | | C3013 | 3.071 | | 7.467 | 1.00 28.5 | | 0 |
| ATOM | 1910 1911 | | | C3013 | 4.533 | | 7.579 | 1.00 28.7 | | 0 |
| ATOM | | | | C3013 | 5.517 | | 6.075 | 1.00 23.3 | | С |
| ATOM | 1912 | C | | | 5.931 | | 5.032 | 1.00 23.4 | | 0 |
| MOTA | 1913 | 0 | | C3013 | 4.855 | | 7.000 | 1.00 23.7 | | N |
| ATOM | 1914 | N | | C3014 | | | 6.818 | 1.00 24.3 | | C |
| ATOM | 1915 | CA | | C3014 | 4.578 | | 8.071 | 1.00 24.9 | | Č |
| ATOM | 1916 | CB | | C3014 | | -10.227 | 9.417 | 1.00 27.0 | | C |
| ATOM | 1917 | CG | | C3014 | | | | 1.00 27.4 | | С |
| MOTA | 1918 | | | C3014 | | -11.044 | 10.423 | 1.00 27.4 | | c |
| MOTA | 1919 | | | C3014 | | -10.589 | 9.258 | | | c |
| MOTA | 1920 | С | | C3014 | 3.660 | | 5.608 | 1.00 24.2 | | 0 |
| MOTA | 1921 | 0 | | C3014 | | -10.939 | 5.004 | 1.00 23.6 | | N |
| MOTA | 1922 | N | | C3015 | 2.857 | | 5.262 | 1.00 24.5 | | |
| ATOM | 1923 | CA | ALA | C3015 | 1.946 | | 4.120 | 1.00 24.9 | | С |
| ATOM | 1924 | CB | | C3015 | 1.082 | | 4.016 | 1.00 25.0 | | C |
| ATOM | 1925 | С | | C3015 | 2.691 | | 2.803 | 1.00 25. | | С |
| ATOM | 1926 | 0 | ALA | C3015 | 2.215 | | 1.940 | 1.00 25.8 | | 0 |
| ATOM | 1927 | N | SER | C3016 | 3.857 | | 2.648 | 1.00 25. | | N |
| ATOM | 1928 | CA | SER | C3016 | 4.658 | | 1.432 | 1.00 25. | | С |
| ATOM | 1929 | CB | SER | C3016 | 5.829 | 7.742 | 1.441 | 1.00 26. | | С |
| ATOM | 1930 | OG | SER | C3016 | 5.385 | | 1.589 | 1.00 27. | | 0 |
| ATOM | 1931 | С | SER | C3016 | 5.204 | -10.159 | 1.275 | 1.00 26. | | С |
| ATOM | 1932 | 0 | SER | C3016 | 5.276 | 5 -10.690 | 0.161 | 1.00 25. | | 0 |
| ATOM | 1933 | N | | C3017 | 5.603 | 3 -10.768 | 2.390 | 1.00 26. | 46 | N |
| ATOM | 1934 | CA | ILE | C3017 | 6.128 | 3 -12.131 | 2.365 | 1.00 26. | 86 | С |
| ATOM | 1935 | CB | | C3017 | 6.839 | 9 -12.474 | 3.706 | 1.00 26. | 57 | С |
| ATOM | 1936 | | | C3017 | 7.30 | 6 -13.925 | 3.709 | 1.00 26. | 15 | С |
| ATOM | 1937 | | | C3017 | 8.029 | 9 -11.526 | 3.923 | 1.00 26. | 30 | С |
| ATOM | 1938 | | | C3017 | 9.10 | 2 -11.612 | 2.842 | 1.00 26. | 29 | С |
| ATOM | 1939 | C | | C3017 | 4.98 | 6 -13.129 | 2.121 | 1.00 28. | 01 | С |
| ATOM | 1940 | Ö | | C3017 | 5.16 | 0 -14.133 | 1.426 | 1.00 27. | 90 | 0 |
| MOTA | 1941 | N | | C3018 | | 6 -12.837 | 2.679 | 1.00 28. | 89 | N |
| ATOM | 1942 | CA | | C3018 | | 7 -13.713 | 2.530 | 1.00 30. | 68 | С |
| ATOM | 1943 | CB | | C3018 | 1.52 | 7 -13.250 | 3.456 | 1.00 31. | 80 | С |
| ATOM | 1944 | CG | | C3018 | | 6 -13.180 | 4.919 | 1.00 32. | 50 | С |
| ATOM | 1945 | CD | | C3018 | | 3 -12.614 | 5.817 | 1.00 33. | 07 | C |
| | | | | C3018 | 0.16 | 1 -11.663 | 5.395 | 1.00 33. | 76 | 0 |
| ATOM | 1947 | | | C3018 | | 4 -13.108 | 6.955 | 1.00 33. | | 0 |
| ATOM | 1948 | | | C3018 | | 4 -13.796 | 1.092 | 1.00 31. | | С |
| | 1940 | | | C3018 | | 6 -14.868 | 0.639 | 1.00 31. | | 0 |
| ATOM | | | | C3019 | | 6 -12.677 | 0.372 | 1.00 32. | | N |
| ATOM | 1950 | | | C3019 | | 1 -12.676 | -1.008 | 1.00 33. | | C |
| MOTA | 1951 1952 | | | C3019 | | 0 -11.240 | -1.494 | 1.00 33 | | С |
| MOTA | | | | C3019 | | 0 -10.547 | -1.838 | 1.00 34 | | 0 |
| ATOM | 1953 | | | C3019 | | 6 -13.364 | -1.918 | 1.00 34 | | С |
| ATOM | 1954 | | | C3019 | | 13.304 | | 1.00 34 | | 0 |
| MOTA | 1955 | | | A C3020 | | 9 -13.191 | | | | N |
| MOTA | 1956 | | | A C3020 | | 51 -13.791 | | | | С |
| ATOM | 1957 | | | A C3020 | | .5 -13.247 | | | | С |
| MOTA | 1958 | CB | ALL | 1 (3020 | 0.41 | .5 15.247 | 2.750 | 2.30 33 | | |

| ATOM | 1959 | С | ALA | C3020 | 5.071 -15.322 -2.347 1.00 36.89 | С |
|--------------|------|------|-----|---------|----------------------------------|---|
| ATOM | 1960 | 0 | ALA | C3020 | 5.451 -15.978 -3.317 1.00 36.66 | 0 |
| MOTA | 1961 | N | VAL | C3021 | 4.663 -15.891 -1.217 1.00 38.20 | N |
| MOTA | 1962 | CA | VAL | C3021 | 4.640 -17.343 -1.078 1.00 40.04 | С |
| ATOM | 1963 | CB | VAL | C3021 | 4.270 -17.770 0.362 1.00 40.00 | С |
| ATOM | 1964 | CG1 | VAL | C3021 | 4.180 -19.285 0.445 1.00 40.22 | С |
| ATOM | 1965 | CG2 | VAL | C3021 | 5.310 -17.255 1.347 1.00 40.17 | С |
| ATOM | 1966 | | | C3021 | 3.636 -17.969 -2.043 1.00 41.37 | С |
| ATOM | 1967 | | | C3021 | 3.939 -18.954 -2.718 1.00 41.44 | 0 |
| ATOM | 1968 | | | C3022 | 2.443 -17.387 -2.105 1.00 42.72 | N |
| ATOM | 1969 | CA | | C3022 | 1.382 -17.883 -2.974 1.00 44.38 | С |
| ATOM | 1970 | СВ | THR | C3022 | 0.049 -17.160 -2.683 1.00 43.84 | С |
| ATOM | 1971 | | | C3022 | -0.341 -17.403 -1.326 1.00 43.59 | 0 |
| ATOM | 1972 | | | C3022 | -1.048 -17.665 -3.612 1.00 43.81 | С |
| ATOM | 1973 | C | | C3022 | 1.703 -17.738 -4.461 1.00 45.84 | С |
| ATOM | 1974 | Ö | | C3022 | 1.725 -18.730 -5.193 1.00 45.92 | 0 |
| ATOM | 1975 | N | | C3023 | 1.951 -16.508 -4.906 1.00 47.48 | N |
| ATOM | 1976 | CA | | C3023 | 2.250 -16.253 -6.313 1.00 49.27 | C |
| ATOM | 1977 | CB | | C3023 | 2.771 -14.823 -6.502 1.00 49.46 | С |
| ATOM | 1978 | CG | | C3023 | 2.801 -14.390 -7.958 1.00 49.98 | С |
| MOTA | 1979 | CD | | C3023 | 2.939 -12.884 -8.125 1.00 50.04 | С |
| ATOM | 1980 | NE | | C3023 | 4.288 -12.399 -7.854 0.05 50.32 | N |
| ATOM | 1981 | CZ | | C3023 | 4.694 -11.158 -8.105 0.05 50.40 | С |
| ATOM | 1982 | | | C3023 | 3.853 -10.279 -8.634 0.05 50.48 | N |
| ATOM | 1983 | | | C3023 | 5.940 -10.797 -7.833 0.05 50.49 | N |
| ATOM | 1984 | C | | C3023 | 3.260 -17.259 -6.861 1.00 50.29 | С |
| | 1985 | 0 | | C3023 | 2.889 -18.186 -7.580 1.00 50.77 | 0 |
| ATOM | 1986 | N | | C3023 | 4.532 -17.074 -6.526 1.00 51.47 | N |
| ATOM ATOM | 1987 | CA | | C3024 | 5.581 -17.988 -6.970 1.00 52.39 | С |
| | 1988 | CB | | C3024 | 6.822 -17.207 -7.410 0.05 52.53 | С |
| ATOM ATOM | 1989 | CG | | C3024 | 7.108 -17.304 -8.876 0.05 52.72 | С |
| ATOM | 1990 | | | C3024 | 7.177 -16.353 -9.838 0.05 52.78 | С |
| ATOM | 1991 | | | C3024 | 7.367 -18.503 -9.505 0.05 52.78 | N |
| ATOM | 1992 | | | C3024 | 7.583 -18.287 -10.790 0.05 52.83 | C |
| ATOM | 1993 | | | C3024 | 7.474 -16.990 -11.018 0.05 52.83 | N |
| ATOM | 1994 | C | | C3024 | 5.931 -18.911 -5.806 1.00 53.02 | С |
| ATOM | 1995 | Ö | | 'C3024 | 6.822 -18.613 -5.013 1.00 52.97 | 0 |
| ATOM | 1996 | N | | C3025 | 5.222 -20.032 -5.712 1.00 53.71 | N |
| ATOM | 1997 | CA | | C3025 | 5.430 -20.992 -4.632 1.00 54.23 | С |
| MOTA | 1998 | СВ | | C3025 | 4.308 -22.035 -4.647 1.00 55.24 | С |
| ATOM | 1999 | CG | | C3025 | 4.150 -22.772 -5.965 1.00 56.63 | С |
| ATOM | 2000 | CD | | C3025 | 2.869 -23.585 -6.024 1.00 57.48 | С |
| ATOM | 2001 | | | C3025 | 2.657 -24.435 -5.131 1.00 58.10 | 0 |
| ATOM | 2002 | | | C3025 | 2.075 -23.372 -6.966 1.00 57.87 | 0 |
| ATOM | 2002 | | | C3025 | 6.796 -21.684 -4.626 1.00 53.75 | С |
| ATOM | 2003 | Ö | | C3025 | 6.916 -22.841 -4.227 1.00 53.95 | 0 |
| ATOM | 2005 | N | | C3026 | 7.820 -20.961 -5.068 1.00 53.15 | N |
| ATOM | 2006 | CA | | C3026 | 9.171 -21.492 -5.080 1.00 51.80 | С |
| MOTA | 2007 | C | | C3026 | 10.057 -20.503 -4.340 1.00 50.97 | C |
| ATOM | 2008 | Ö | | C3026 | 11.260 -20.712 -4.167 1.00 50.85 | 0 |
| ATOM | 2009 | | | C3027 | 9.426 -19.418 -3.899 1.00 49.86 | N |
| ATOM | 2010 | CA | | C3027 | 10.077 -18.331 -3.173 1.00 48.78 | С |
| ATOM | 2010 | | | C3027 | 9.001 -17.419 -2.570 1.00 48.81 | С |
| ATOM | 2011 | | | C3027 | 9.546 -16.198 -1.884 1.00 48.66 | С |
| ATOM | 2012 | | | C3027 | 10.279 -15.252 -2.593 1.00 48.61 | C |
| ATOM | 2013 | | | C3027 | 9.313 -15.986 -0.527 1.00 48.69 | С |
| ATOM | 2014 | | | C3027 | 10.772 -14.111 -1.962 1.00 48.58 | С |
| ATON | 2013 | Ų L. | 111 | _ 00027 | ##**** | |

| ATOM | 2016 | CE2 | PHE | C3027 | 9.802 -14.849 | 0.113 | 1.00 48.35 | С |
|------|--------|-----|-----|---------|----------------|-----------|------------|-----|
| ATOM | 2017 | | | C3027 | 10.533 -13.910 | | 1.00 48.38 | С |
| ATOM | 2018 | C | | C3027 | 11.037 -18.795 | | 1.00 47.88 | С |
| ATOM | 2019 | 0 | | C3027 | 12.188 -18.364 | | 1.00 47.77 | 0 |
| ATOM | 2020 | | | C3028 | 10.558 -19.676 | | 1.00 47.03 | N |
| ATOM | 2020 | CA | | C3028 | 11.362 -20.186 | | 1.00 46.36 | c |
| | 2021 | | | C3028 | 10.529 -21.147 | | 1.00 46.30 | Č |
| ATOM | | | | C3028 | 12.668 -20.862 | | 1.00 45.98 | . c |
| ATOM | 2023 | | | | 13.735 -20.562 | | 1.00 46.02 | Ö |
| ATOM | 2024 | | | C3028 | | | 1.00 44.97 | N |
| ATOM | 2025 | N | | C3029 | 12.585 -21.774 | | 1.00 44.02 | C |
| ATOM | 2026 | CA | | C3029 | 13.762 -22.497 | | 1.00 44.02 | C |
| MOTA | 2027 | CB | | C3029 | 13.377 -23.478 | | 0.05 44.27 | c |
| MOTA | 2028 | CG | | C3029 | 12.440 -24.589 | | | |
| MOTA | 2029 | CD | | C3029 | 12.186 -25.576 | | 0.05 44.38 | C |
| ATOM | 2030 | CE | | C3029 | 11.290 -26.717 | | 0.05 44.42 | |
| MOTA | 2031 | NZ | | C3029 | 11.066 -27.712 | | 0.05 44.48 | N |
| ATOM | 2032 | С | LYS | C3029 | 14.878 -21.586 | | 1.00 43.30 | С |
| MOTA | 2033 | 0 | | C3029 | 16.055 -21.926 | • | 1.00 43.66 | 0 |
| ATOM | 2034 | N | ARG | C3030 | 14.516 -20.429 | | 1.00 42.33 | N |
| MOTA | 2035 | CA | ARG | C3030 | 15.515 -19.498 | 3 -3.495 | 1.00 41.38 | С |
| ATOM | 2036 | CB | ARG | C3030 | 14.933 -18.685 | -4.655 | 1.00 41.73 | С |
| ATOM | 2037 | CG | ARG | C3030 | 14.577 -19.52 | 7 -5.870 | 0.05 41.77 | С |
| ATOM | 2038 | CD | ARG | C3030 | 14.062 -18.672 | 2 -7.016 | 0.05 41.90 | С |
| ATOM | 2039 | NE | ARG | C3030 | 13.773 -19.47 | 4 -8.202 | 0.05 42.00 | N |
| ATOM | 2040 | CZ | | C3030 | 13.329 -18.97 | 7 -9.351 | 0.05 42.04 | С |
| ATOM | 2041 | | | C3030 | 13.092 -19.78 | 4 -10.377 | 0.05 42.08 | N |
| ATOM | 2042 | | | C3030 | 13.119 -17.67 | | 0.05 42.08 | N |
| ATOM | 2043 | C | | C3030 | 16.073 -18.55 | | 1.00 40.66 | С |
| ATOM | 2044 | Ö | | C3030 | 17.141 -17.96 | | 1.00 40.56 | 0 |
| ATOM | 2045 | N | | C3031 | 15.357 -18.40 | | 1.00 39.61 | N |
| ATOM | 2046 | CA | | C3031 | 15.797 -17.50 | | 1.00 38.51 | С |
| ATOM | 2047 | CB | | C3031 | 14.593 -16.73 | | 1.00 38.68 | С |
| ATOM | 2048 | | | C3031 | 15.046 -15.89 | | 1.00 39.01 | С |
| | 2048 | | | C3031 | 13.964 -15.84 | | 1.00 39.32 | С |
| MOTA | | C | | C3031 | 16.535 -18.22 | | 1.00 37.22 | C |
| ATOM | 2050 | | | C3031 | 17.392 -17.62 | | 1.00 36.96 | 0 |
| ATOM | 2051 | 0 | | | 16.215 -19.49 | | 1.00 35.97 | N |
| ATOM | 2052 | N | | C3032 | 16.825 -20.26 | | 1.00 35.20 | Ċ |
| ATOM | 2053 | CA | | C3032 | 15.713 -20.86 | | 1.00 34.43 | Ċ |
| ATOM | 2054 | CB | | C3032 | 14.682 -19.88 | | 1.00 34.43 | Ċ |
| MOTA | 2055 | CG | | C3032 | | | 1.00 34.07 | C |
| ATOM | 2056 | | | C3032 | 13.508 -20.65 | | | Č |
| ATOM | 2057 | | | C3032 | 15.340 -19.01 | | | c |
| ATOM | 2058 | С | | C3032 | 17.774 -21.39 | | | Õ |
| ATOM | 2059 | 0 | | C3032 | 17.592 -21.99 | | | N |
| ATOM | 2060 | N | | C3033 | 18.780 -21.67 | | 1.00 34.45 | C |
| ATOM | 2061 | CA | | C3033 | 19.729 -22.75 | | | |
| ATOM | 2062 | CB | | C3033 | 21.050 -22.61 | | | С |
| MOTA | 2063 | | | C3033 | 20.797 -22.88 | | | 0 |
| ATOM | 2064 | CG2 | | C3033 | 21.630 -21.22 | | | C |
| MOTA | 2065 | С | | C3033 | 19.063 -24.06 | | | С |
| MOTA | 2066 | 0 | | C3033 | 17.968 -24.05 | | | 0 |
| ATOM | 2067 | N | | C3034 | 19.729 -25.18 | | | N |
| MOTA | 2068 | CA | | C3034 | 19.178 -26.48 | | | C |
| MOTA | 2069 | CB | | A C3034 | 20.103 -27.59 | | | C |
| ATOM | 2070 | C | | A C3034 | 18.927 -26.63 | | | C |
| ATOM | - 2071 | 0 | | A C3034 | 17.867 -27.11 | | | . 0 |
| ATOM | 2072 | N | LEU | J C3035 | 19.895 -26.23 | 33 5.162 | 1.00 34.52 | N |
| | | | | | | | | |

| ATOM | 2073 | CA | LEU | C3035 | 19.755 | -26.345 | 6.612 | 1.00 | 34.61 | | С |
|--------|------|-----|-----|---------|--------|-------------|--------|-------|---------|---|--------|
| ATOM | 2074 | | | C3035 | 21.087 | 7 -26.047 | 7.308 | 1.00 | 34.52 | | С |
| ATOM | 2075 | CG | | C3035 | 21.103 | L -26.182 | 8.834 | 0.05 | | | С |
| ATOM | 2076 | | | C3035 | | 1 -27.607 | 9.228 | 0.05 | 34.51 | | С |
| ATOM | 2077 | | | C3035 | 22.47 | 5 -25.814 | 9.369 | 0.05 | 34.53 | | С |
| ATOM | 2078 | С | | C3035 | | 5 -25.414 | 7.156 | 1.00 | | | С |
| ATOM | 2079 | 0 | | C3035 | | 5 -25.769 | 8.098 | 1.00 | 35.04 | | 0 |
| ATOM | 2080 | N | | C3036 | 18.55 | 8 -24.222 | 6.574 | 1.00 | 35.33 | | N |
| ATOM | 2081 | CA | | C3036 | | 7 -23.263 | 7.004 | 1.00 | 35.62 | | С |
| MOTA | 2082 | CB | | C3036 | 17.74 | 1 -21.907 | 6.310 | 1.00 | 34.70 | | С |
| ATOM | 2083 | CG | | C3036 | 18.80 | 9 -21.006 | 6.941 | 1.00 | 33.21 | | С |
| ATOM | 2084 | CD | | C3036 | | 7 -19.767 | 6.103 | 1.00 | 32.82 | | С |
| ATOM | 2085 | | GLU | C3036 | 19.59 | 8 -18.759 | 6.671 | 1.00 | 31.24 | | 0 |
| ATOM | 2086 | OE2 | GLU | C3036 | 18.89 | 3 -19.803 | 4.873 | 1.00 | 32.21 | | 0 |
| ATOM | 2087 | C | | C3036 | | 5 -23.815 | 6.654 | 1.00 | 36.75 | | С |
| ATOM | 2088 | Ō | | C3036 | 15.20 | 5 -23.687 | 7.427 | | 36.40 | | 0 |
| ATOM | 2089 | N | MET | C3037 | 16.06 | 4 -24.436 | 5.481 | 1.00 | 38.24 | | N |
| ATOM | 2090 | CA | MET | C3037 | | 1 -25.018 | 4.981 | | 40.09 | | С |
| ATOM | 2091 | CB | MET | C3037 | 15.06 | 4 -25.625 | 3.596 | | 41.14 | | С |
| ATOM | 2092 | CG | | C3037 | 13.80 | 8 -26.028 | 2.834 | | 43.15 | | С |
| ATOM | 2093 | SD | MET | C3037 | 12.85 | 1 -24.618 | 2.239 | 1.00. | 45.06 | | S |
| ATOM | 2094 | CE | MET | C3037 | 11.18 | 9 -25.242 | 2.400 | 1.00 | 44.92 | • | С |
| ATOM | 2095 | С | MET | C3037 | 14.27 | 0 -26.089 | 5.926 | | 40.63 | • | С |
| ATOM | 2096 | 0 | MET | C3037 | 13.06 | 1 -26.171 | 6.151 | | 40.94 | | 0 |
| ATOM | 2097 | N | | C3038 | 15.15 | 9 -26.911 | 6.473 | 1.00 | 41.23 | | N |
| ATOM | 2098 | CA | GLU | C3038 | 14.75 | 2 -27.969 | 7.393 | 1.00 | 41.49 | | С |
| ATOM | 2099 | CB | GLU | C3038 | 15.98 | 2 -28.713 | 7.924 | 1.00 | 41.61 | | C |
| ATOM | 2100 | CG | GLU | C3038 | 16.71 | 1 -29.544 | 6.878 | 0.05 | 41.50 | | C |
| ATOM | 2101 | CD | | C3038 | 15.88 | 9 -30.721 | 6.385 | 0.05 | 41.51 | | С |
| ATOM | 2102 | | GLU | C3038 | 16.37 | 6 -31.459 | 5.503 | | 41.48 | | 0 |
| ATOM | 2103 | | | C3038 | 14.75 | 8 -30.911 | 6.880 | 0.05 | 41.45 | | 0 |
| ATOM | 2104 | С | | C3038 | 13.95 | 8 -27.391 | 8.559 | | 41.78 | | C |
| ATOM | 2105 | 0 | GLU | C3038 | | 34 -27.989 | 9.013 | | 41.81 | | 0 |
| ATOM | 2106 | N | ARG | C3039 | | 34 -26.226 | 9.037 | | 42.11 | | N |
| ATOM | 2107 | CA | ARG | C3039 | | L6 -25.550 | 10.146 | | 42.69 | | C |
| MOTA | 2108 | CB | ARG | C3039 | | 30 -24.380 | 10.634 | | 43.67 | | C |
| MOTA | 2109 | CG | ARG | C3039 | | 50 -23.514 | 11.722 | | 45.06 | | С |
| ATOM | 2110 | CD | ARG | C3039 | | 52 -24.276 | 13.026 | | 46.69 | | C |
| ATOM | 2111 | NE | ARG | C3039 | | 95 -23.394 | 14.099 | | 47.90. | | N |
| MOTA | 2112 | CZ | ARG | C3039 | | 66 -23.803 | 15.321 | | 48.72 | | C |
| ATOM | 2113 | NH1 | ARC | G C3039 | | 4.0 -25.089 | 15.637 | | 49.17 | | N |
| ATOM | 2114 | NH2 | ARC | G C3039 | | 63 -22.925 | 16.230 | | 49.02 | | N |
| MOTA | 2115 | С | ARC | G C3039 | | 43 -25.034 | 9.714 | | 42.44 | | C |
| MOTA | 2116 | 0 | | G C3039 | | 60 -25.153 | 10.448 | | 42.21 | | 0 |
| ATOM | 2117 | N | | E C3040 | | 93 -24.467 | 8.512 | | 42.44 | | N |
| ATOM | 2118 | CA | PHI | E C3040 | | 64 -23.909 | 7.948 | | 42.58 | | C |
| MOTA | 2119 | CB | | E C3040 | | 43 -23.394 | 6.529 | | 41.84 | | C |
| ATOM | 2120 | CG | | E C3040 | | 65 -22.713 | 5.879 | | 41.26 | | C |
| ATOM | 2121 | | | E C3040 | | 21 -21.556 | 6.428 | | 40.76 | | |
| ATOM | 2122 | | | E C3040 | | 10 -23.223 | 4.708 | | 40.96 | | C |
| ATOM | 2123 | | | E C3040 | | 41 -20.915 | 5.821 | | 40.74 | | C C |
| MOTA | 2124 | | | E C3040 | | 27 -22.590 | 4.090 | | 40.92 | | C |
| ATOM | 2125 | | | E C3040 | | 92 -21.433 | 4.649 | | 40.88 | | C |
| MOTA | 2126 | | | E C3040 | | 99 -24.902 | 7.913 | | 3 43.12 | • | 0 |
| MOTA | 2127 | | | E C3040 | | 90 -24.585 | 8.343 | | 1 42.92 | | N |
| MOTA | 2128 | | | R C3041 | | .56 -26.104 | 7.406 | | 3 43.77 | | C |
| MOTA · | 2129 | CA | TH | R C3041 | 9.1 | 19 -27.126 | 7.303 | 1.00 | 0 44.43 | | C |

| | | | | | | | | | 1 00 | 44.00 | _ |
|------|------|-----|-------|---------|------------|-------|-----------|--------|------|---------|---|
| MOTA | 2130 | CB | | C3041 | | | -28.283 | 6.395 | | 44.80 | С |
| MOTA | 2131 | OGI | THR | C3041 | | | -28.936 | 6.978 | | 45.05 | 0 |
| ATOM | 2132 | CG2 | THR | C3041 | | | -27.759 | 5.016 | | 45.00 | C |
| ATOM | 2133 | С | THR | C3041 | | | -27.719 | 8.635 | | 44.57 | С |
| ATOM | 2134 | 0 | THR | C3041 | | | -28.327 | 8.721 | | 44.92 | 0 |
| MOTA | 2135 | N | SER | C3042 | 9. | 488 | -27.548 | 9.672 | | 44.91 | N |
| ATOM | 2136 | CA | SER | C3042 | | | -28.091 | 10.986 | | 44.98 | C |
| ATOM | 2137 | CB | SER | C3042 | | | -28.297 | 11.801 | | 45.18 | С |
| ATOM | 2138 | OG | SER | C3042 | 11. | 336 | -29.151 | 11.110 | 1.00 | 45.91 | 0 |
| ATOM | 2139 | С | SER | C3042 | 8. | 194 | -27.212 | 11.770 | | 44.99 | С |
| ATOM | 2140 | 0 | | C3042 | 7. | 536 | -27.683 | 12.699 | 1.00 | 45.11 | 0 |
| ATOM | 2141 | N | | C3043 | 8. | 112 | -25.938 | 11.397 | 1.00 | 44.68 | N |
| ATOM | 2142 | CA | | C3043 | | | -24.993 | 12.073 | 1.00 | 44.47 | С |
| ATOM | 2143 | СВ | | C3043 | | | -23.608 | 12.124 | 1.00 | 44.33 | С |
| ATOM | 2144 | CG | | C3043 | | | -23.485 | 12.797 | 1.00 | 44.21 | С |
| ATOM | 2145 | | | C3043 | | | -22.052 | 12.662 | 1.00 | 44.22 | С |
| ATOM | 2146 | | | C3043 | | | -23.875 | 14.265 | 1.00 | 44.47 | С |
| ATOM | 2147 | C | | C3043 | | | -24.899 | 11.347 | 1.00 | 44.31 | С |
| | 2148 | 0 | | C3043 | | | -25.422 | 10.240 | 1.00 | 44.09 | 0 |
| ATOM | 2149 | N | | C3044 | | | -24.221 | 11.965 | 1.00 | 44.27 | N |
| ATOM | | | | C3044 | | | -24.064 | 11.365 | | 44.15 | С |
| ATOM | 2150 | CA | | C3044 | | | -25.234 | 11.777 | | 45.11 | С |
| MOTA | 2151 | CB | | | | | -25.375 | 10.953 | | 46.10 | С |
| MOTA | 2152 | CG | | C3044 | | | -26.398 | 11.547 | | 47.10 | C |
| MOTA | 2153 | CD | | C3044 | | | -27.774 | 11.701 | | 47.88 | C |
| ATOM | 2154 | CE | | C3044 | | | | 12.758 | | 48.36 | N |
| ATOM | 2155 | NZ | | C3044 | | | -27.802 | 11.753 | | 43.58 | Ċ |
| ATOM | 2156 | С | | C3044 | | | -22.745 | | | 43.58 | Ö |
| ATOM | 2157 | 0 | | C3044 | | | -22.062 | 12.687 | | 42.72 | N |
| ATOM | 2158 | N | | C3045 | | | -22.397 | 11.022 | | 41.65 | C |
| ATOM | 2159 | CA | | C3045 | | | -21.177 | 11.299 | | 40.64 | Ċ |
| MOTA | 2160 | С | | C3045 | | | -19.893 | 11.197 | | 40.57 | Ö |
| ATOM | 2161 | 0 | | C3045 | | | -19.749 | 10.323 | | 39.78 | N |
| MOTA | 2162 | N | | C3046 | | | -18.956 | 12.097 | | | C |
| MOTA | 2163 | CA | | C3046 | | | -17.666 | 12.129 | | 38.64 | c |
| ATOM | 2164 | CB | | C3046 | | | -16.792 | 13.249 | | 38.93 | c |
| MOTA | 2165 | CG | | G C3046 | | | -15.415 | 13.350 | | 38.89 | C |
| MOTA | 2166 | CD | ARC | G C3046 | | | -14.591 | 14.465 | | 38.99 | N |
| MOTA | 2167 | NE | | G C3046 | | | -14.352 | 14.241 | | 39.04 | |
| MOTA | 2168 | CZ | | G C3046 | | | -13.636 | 15.050 | | 39.08 | C |
| ATOM | 2169 | NHI | . ARC | G C3046 | | | -13.471 | 14.768 | | 39.09 | N |
| MOTA | 2170 | NH2 | 2 ARG | G C3046 | | | -13.084 | 16.142 | | 39.12 | N |
| MOTA | 2171 | С | | G C3046 | | | -17.840 | 12.338 | | 37.81 | С |
| ATOM | 2172 | 0 | ARG | G C3046 | | | -17.130 | 11.735 | | 37.34 | 0 |
| ATOM | 2173 | N | | G C3047 | 4 | .195 | -18.785 | 13.198 | | 36.94 | N |
| MOTA | 2174 | CA | AR | G C3047 | | | -19.056 | 13.485 | 1.00 | 35.80 | C |
| MOTA | 2175 | | AR | G C3047 | | | -20.255 | 14.424 | | 37.34 | С |
| ATOM | 2176 | CG | AR | G C3047 | | | -19.924 | 15.887 | | 38.72 | C |
| MOTA | 2177 | CD | AR | G C3047 | | | -21.177 | 16.731 | | 40.55 | C |
| ATOM | 2178 | NE | | G C3047 | | | -20.870 | 18.083 | | 0 41.86 | N |
| ATOM | 2179 | | | G C3047 | | | -20.335 | 18.369 | | 0 42.33 | C |
| ATOM | 2180 | | | G C3047 | | | -20.050 | 17.395 | | 0 43.10 | N |
| ATOM | 2181 | | 2 AR | G C3047 | | | -20.087 | 19.629 | | 0 42.88 | N |
| ATOM | 2182 | | | G C3047 | ϵ | .408 | -19.329 | 12.223 | | 0 34.36 | С |
| ATOM | 2183 | | | G C3047 | 7 | .518 | -18.812 | 12.057 | | 0 33.67 | 0 |
| ATOM | 2184 | | GL | N C3048 | | | 2 -20.152 | | | 0 32.32 | N |
| ATOM | 2185 | | | N C3048 | (| 5.522 | 2 -20.493 | | | 0 30.19 | С |
| ATOM | 2186 | | | N C3048 | 5 | .709 | 9 -21.538 | 9.326 | 1.0 | 0 3056 | С |
| | | | | | | | | | | | |

| ATOM | 2187 | CG | GLN | C3048 | 6.346 | -21.947 | 8.010 | 1.00 31.08 | С |
|------|------|-----|-----|-------|---------|-----------------|--------|------------|-----|
| ATOM | 2188 | CD | GLN | C3048 | • 5.545 | -22.989 | 7.256 | 1.00 31.55 | С |
| MOTA | 2189 | OEI | GLN | C3048 | 4.363 | -22.793 | 6.971 | 1.00 32.61 | 0 |
| ATOM | 2190 | NE2 | GLN | C3048 | 6.189 | -24.100 | 6.919 | 1.00 31.23 | N |
| ATOM | 2191 | С | GLN | C3048 | 6.749 | -19.266 | 9.211 | 1.00 28.78 | С |
| MOTA | 2192 | 0 | GLN | C3048 | 7.816 | -19.113 | 8.615 | 1.00 27.77 | 0 |
| MOTA | 2193 | N | ILE | C3049 | 5.747 | -18.396 | 9.124 | 1.00 27.16 | N |
| ATOM | 2194 | CA | ILE | C3049 | 5.862 | -17.195 | 8.298 | 1.00 26.51 | С |
| MOTA | 2195 | CB | | C3049 | 4.485 | - 16.521 | 8.086 | 1.00 26.30 | С |
| MOTA | 2196 | CG2 | ILE | C3049 | 4.647 | -15.250 | 7.255 | 1.00 26.17 | С |
| ATOM | 2197 | CG1 | ILE | C3049 | 3.530 | -17.491 | 7.380 | 1.00 26.22 | С |
| ATOM | 2198 | CD1 | ILE | C3049 | 4.023 | -17.978 | 6.014 | 1.00 26.61 | С |
| MOTA | 2199 | С | ILE | C3049 | 6.831 | -16.178 | 8.910 | 1.00 25.94 | С |
| ATOM | 2200 | 0 | | C3049 | 7.570 | -15.510 | 8.192 | 1.00 25.27 | 0 |
| ATOM | 2201 | N | | C3050 | 6.824 | -16.069 | 10.236 | 1.00 26.02 | N |
| ATOM | 2202 | CA | | C3050 | | -15.141 | 10.935 | 1.00 25.96 | С |
| ATOM | 2203 | СВ | | C3050 | | -15.075 | 12.423 | 1.00 27.39 | С |
| ATOM | 2204 | CG | | C3050 | | -14.287 | 12.724 | 1.00 29.92 | · c |
| ATOM | 2205 | CD | | C3050 | | -12.853 | 13.175 | 1.00 31.52 | С |
| ATOM | 2206 | | | C3050 | | -12.322 | 12.894 | 1.00 32.57 | 0 |
| ATOM | 2207 | | | C3050 | | -12.252 | 13.802 | 1.00 31.86 | 0 |
| ATOM | 2208 | C | | C3050 | | -15.521 | 10.792 | 1.00 24.88 | С |
| ATOM | 2209 | ŏ | | C3050 | | -14.650 | 10.815 | 1.00 24.17 | Ō |
| ATOM | 2210 | N | | C3051 | | -16.815 | 10.652 | 1.00 23.54 | N |
| ATOM | 2211 | CA | | C3051 | | -17.281 | 10.508 | 1.00 22.59 | С |
| ATOM | 2212 | CB | | C3051 | | -18.808 | 10.711 | 1.00 23.12 | C |
| ATOM | 2213 | CG | | C3051 | | -19.425 | 10.473 | 1.00 23.17 | C |
| ATOM | 2214 | | | C3051 | | -19.902 | 9.213 | 1.00 23.85 | C |
| ATOM | 2215 | | | C3051 | | -20.454 | 8.984 | 1.00 24.32 | c |
| ATOM | 2216 | | | C3051 | | -19.515 | 11.504 | 1.00 24.30 | c |
| ATOM | 2217 | | | C3051 | | -20.064 | 11.288 | 1.00 24.54 | C |
| ATOM | 2218 | CZ | | C3051 | | -20.528 | 10.026 | 1.00 24.99 | c |
| ATOM | 2219 | OH | | C3051 | | -21.050 | 9.803 | 1.00 25.78 | 0 |
| ATOM | 2220 | C | | C3051 | | -16.894 | 9.140 | 1.00 22.18 | С |
| ATOM | 2221 | 0 | | C3051 | | -16.395 | 9.031 | 1.00 20.97 | Ō |
| ATOM | 2222 | N | | C3052 | | -17.115 | 8.101 | 1.00 21.39 | N |
| ATOM | 2223 | CA | | C3052 | | -16.787 | 6.736 | 1.00 21.55 | С |
| ATOM | 2224 | CB | | C3052 | | -17.254 | 5.747 | 1.00 22.13 | C |
| ATOM | 2225 | CG | | C3052 | | -16.929 | 4.259 | 1.00 21.93 | С |
| ATOM | 2226 | | | C3052 | | -17.515 | 3.755 | 1.00 22.55 | С |
| ATOM | 2227 | | | C3052 | | -17.495 | 3.469 | 1.00 22.75 | C |
| ATOM | 2228 | C | | C3052 | | -15.284 | 6.574 | 1.00 21.31 | C |
| ATOM | 2229 | Ō | | C3052 | | -14.866 | 5.914 | 1.00 21.85 | 0 |
| MOTA | 2230 | N | | C3053 | | -14.484 | 7.181 | 1.00 20.68 | N |
| ATOM | 2231 | CA | | C3053 | | -13.025 | 7.102 | 1.00 20.75 | С |
| ATOM | 2232 | CB | | C3053 | | 3 -12.401 | 7.738 | 1.00 20.99 | С |
| MOTA | 2233 | C | | C3053 | | -12.469 | 7.768 | 1.00 20.60 | С |
| ATOM | 2234 | 0 | | C3053 | | 5 -11.552 | 7.237 | 1.00 20.36 | 0 |
| ATOM | 2235 | N | | C3054 | | 3 -13.027 | 8.925 | 1.00 20.45 | N |
| ATOM | 2236 | CA | | C3054 | | -12.597 | 9.646 | 1.00 20.63 | С |
| ATOM | 2237 | C | | C3054 | | 5 -12.928 | 8.945 | 1.00 20.53 | С |
| ATOM | 2238 | Ō | | C3054 | | -12.174 | 9.034 | 1.00 19.61 | 0 |
| ATOM | 2239 | N | | C3055 | | -14.065 | 8.256 | 1.00 20.88 | N |
| ATOM | 2240 | CA | | C3055 | | 4 -14.457 | 7.527 | 1.00 21.09 | С |
| ATOM | 2241 | CB | | C3055 | | 1 -15.930 | 7.101 | 1.00 21.81 | C |
| ATOM | 2242 | CG | ARG | C3055 | | 3 -16.895 | 7.988 | 1.00 23.24 | С |
| ATOM | 2243 | CD | ARG | C3055 | 16.13 | 9 -16.801 | 9.465 | 1.00 23.82 | С |
| | | | | | | | | | |

| ATOM | 2244 | NE | ARG | C3055 | 17.018 | -17.600 | 10.325 | 1.00 23.91 | N |
|--------------|--------------|----------|-----|----------------|------------------|--------------------|----------------|------------|---|
| MOTA | 2245 | CZ | ARG | C3055 | 16.881 | -17.706 | 11.646 | 1.00 24.64 | C |
| ATOM | 2246 | NH1 | ARG | C3055 | 15.901 | -17.065 | 12.267 | 1.00 23.93 | N |
| MOTA | 2247 | NH2 | ARG | C3055 | 17.719 | -18.459 | 12.352 | 1.00 25.21 | N |
| ATOM | 2248 | С | ARG | C3055 | 16.017 | -13.552 | 6.301 | 1.00 21.23 | С |
| ATOM | 2249 | 0 | ARG | C3055 | 17.142 | -13.234 | 5,921 | 1.00 20.84 | 0 |
| MOTA | 2250 | N | TRP | C3056 | 14.911 | -13.132 | 5.694 | 1.00 21.62 | N |
| MOTA | 2251 | CA | TRP | C3056 | 14.958 | -12.247 | 4.529 | 1.00 22.92 | С |
| ATOM | 2252 | СВ | | C3056 | | -12.121 | 3.910 | 1.00 25.18 | С |
| ATOM | 2253 | CG | | C3056 | | -11.388 | 2.594 | 1.00 27.65 | C |
| ATOM | 2254 | | | C3056 | 13.357 | -9.977 | 2.401 | 1.00 28.51 | С |
| ATOM | 2255 | | | C3056 | 13.413 | -9.736 | 1.009 | 1.00 29.11 | C |
| ATOM | 2256 | | | C3056 | 13.176 | -8.892 | 3.269 | 1.00 29.11 | С |
| ATOM | 2257 | | | C3056 | | -11.931 | 1.344 | 1.00 28.78 | С |
| ATOM | 2258 | | | C3056 | | -10.944 | 0.388 | 1.00 29.88 | N |
| ATOM | 2259 | | | C3056 | 13.296 | -8.453 | 0.465 | 1.00 28.95 | С |
| ATOM | 2260 | | | C3056 | 13.060 | -7.614 | 2.726 | 1.00 29.68 | C |
| ATOM | 2261 | | | C3056 | 13.121 | -7.409 | 1.336 | 1.00 29.31 | Ĉ |
| ATOM | 2262 | C | | C3056 | | -10.855 | 4.953 | 1.00 22.17 | C |
| ATOM | 2263 | 0 | | C3056 | | -10.247 | 4.281 | 1.00 22.33 | ō |
| ATOM | 2264 | N | | C3057 | | -10.365 | 6.078 | 1.00 21.01 | N |
| ATOM | 2265 | CA | | C3057 | 15.311 | -9.041 | 6.587 | 1.00 20.66 | C |
| ATOM | 2266 | CB | | C3057 | 14.388 | -8.663 | 7.751 | 1.00 21.23 | c |
| ATOM | 2267 | OG | | C3057 | 14.569 | -7.311 | 8.147 | 1.00 22.78 | Ö |
| ATOM | 2268 | C | | C3057 | 16.786 | -8.969 | 7.025 | 1.00 20.18 | C |
| | | | | C3057 | 17.464 | -7.959 | 6.803 | 1.00 20.10 | 0 |
| ATOM | 2269 | 0 | | | 17.280 | | 7.633 | 1.00 18.66 | N |
| ATOM | 2270 | N | | C3058 | | -10.043 | 8.085 | 1.00 18.83 | C |
| ATOM | 2271 | CA | | C3058 | | -11.344 | 8.939 | 1.00 17.30 | C |
| ATOM | 2272 | CB | | C3058 | | -10.062 | 6.915 | 1.00 17.30 | C |
| ATOM | 2273 | С | | C3058 | 20.693 | -9.381 | 6.980 | 1.00 18.44 | 0 |
| ATOM | 2274 | 0 | | C3058 | | -10.803 | 5.851 | 1.00 18.60 | N |
| ATOM | 2275 | N | | C3059 | | | 4.692 | 1.00 18.76 | c |
| ATOM | 2276 | CA | | C3059 | | -10.850 | 3.766 | 1.00 18.70 | C |
| ATOM | 2277 | CB | | C3059 | | -12.012 -13.396 | | 1.00 18.86 | c |
| ATOM | 2278 | CG | | C3059 | | | 4.447 3.494 | 1.00 19.28 | c |
| ATOM | 2279 | CD | | C3059 | | -14.578 -15.920 | 4.244 | 1.00 19.20 | C |
| ATOM | 2280 | CE | | C3059 | | | 3.388 | 1.00 20.00 | И |
| ATOM | 2281 | ΝZ | | C3059 | | -17.130 | | 1.00 20.93 | C |
| ATOM | 2282 | C | | C3059 | 20.274 | -9.508 | 3.938 | | 0 |
| ATOM ATOM | 2283 | 0 | | C3059 C3060 | 21.306 19.142 | -9.117 -8.804 | 3.388 3.935 | 1.00 20.13 | N |
| | 2284 | N | | | 19.026 | -7.501 | 3.277 | 1.00 20.20 | C |
| ATOM | 2285 | CA | | C3060 | 17.550 | | 3.205 | 1.00 20.93 | C |
| ATOM | 2286 | CB | | C3060 C3060 | 17.268 | -7.090 -5.739 | 2.545 | 1.00 25.10 | c |
| MOTA | | · CG | | C3060 | 17.579 | -5.738 -5.717 | 1.055 | 1.00 20.03 | c |
| ATOM | 2288 2289 | | | C3060 | 17.161 | -6.660 | 0.341 | 1.00 29.37 | 0 |
| ATOM | 2290 | | | C3060 | 18.232 | -4.749 | 0.598 | 1.00 30.70 | ő |
| MOTA MOTA | 2291 | | | C3060 | 19.837 | -6.432 | 4.030 | 1.00 20.53 | č |
| | 2292 | C | | C3060 | 20.455 | ~5.563 | 3.414 | 1.00 20.33 | o |
| ATOM | 2292 | 0 | | C3060 | 19.838 | -6.497 | 5.360 | 1.00 20.20 | N |
| ATOM | | N | | | | | 6.165 | 1.00 19.74 | C |
| ATOM | 2294 | CA | | C3061 C3061 | 20.591 20.252 | ~5.531 ~5.696 | 7.656 | 1.00 19.24 | c |
| MOTA MOTA | 2295 | СВ | | | 20.252 | -5.711 | 5.938 | 1.00 19.62 | C |
| | 2296 2297 | С | | C3061 C3061 | | -4.732 | 5.885 | 1.00 18.37 | 0 |
| ATOM | | 0 | | C3061 | 22.848 22.530 | | 5.811 | 1.00 18.37 | И |
| ATOM | 2298 | N | | C3062 | 23.941 | -7.270 | 5.570 | 1.00 18.75 | C |
| ATOM ATOM | 2299 2300 | CA CB | | C3062 | 24.190 | | 5.714 | 1.00 19.03 | C |
| WI OU | 2300 | CD | EHE | C300Z | 24.130 | -0.703 | 0.114 | 1.00 19.70 | 0 |

| ATOM | 2301 | CG | | C3062 | 25.592 | -9.224 | 5.325 | 1.00 20.12 | C |
|--------------|------|-----|-------|-------|--------|-----------|--------|------------|-----|
| ATOM | 2302 | | | C3062 | 25.917 | -9.472 | 3.988 | 1.00 20.55 | C |
| MOTA | 2303 | | | C3062 | 26.577 | -9.391 | 6.293 | 1.00 20.19 | С |
| MOTA | 2304 | | | C3062 | 27.200 | -9.883 | 3.622 | 1.00 21.03 | C |
| MOTA | 2305 | CE2 | | C3062 | 27.871 | -9.803 | 5.940 | 1.00 20.44 | C |
| ATOM | 2306 | CZ | | C3062 | 28.181 | -10.049 | 4.598 | 1.00 20.96 | С |
| MOTA | 2307 | C | PHE | C3062 | 24.381 | -6.784 | 4.182 | 1.00 20.13 | С |
| ATOM | 2308 | 0 | PHE | C3062 | 25.474 | -6.231 | 4.037 | 1.00 20.04 | 0 |
| ATOM | 2309 | N | SER | C3063 | 23.530 | -6.981 | 3.174 | 1.00 21.29 | N |
| ATOM | 2310 | CA | SER | C3063 | 23.840 | -6.551 | 1.808 | 1.00 22.13 | С |
| ATOM | 2311 | CB | SER | C3063 | 22.727 | -6.967 | 0.832 | 1.00 22.59 | С |
| ATOM | 2312 | OG | SER | C3063 | 22.699 | -8.374 | 0.636 | 1.00 24.36 | 0 |
| ATOM | 2313 | С | SER | C3063 | 24.019 | -5.032 | 1.762 | 1.00 22.61 | С |
| ATOM | 2314 | 0 | SER | C3063 | 24.913 | -4.527 | 1.082 | 1.00 22.10 | 0 |
| ATOM | 2315 | N | LYS | C3064 | 23.160 | -4.309 | 2.477 | 1.00 22.80 | N |
| ATOM | 2316 | CA | LYS | C3064 | 23.257 | -2.852 | 2.530 | 1.00 24.07 | С |
| MOTA | 2317 | CB | LYS | C3064 | 22.013 | -2.261 | 3,210 | 1.00 23.92 | C |
| MOTA | 2318 | CG | LYS | C3064 | 20.734 | -2.376 | 2.377 | 1.00 23.95 | С |
| ATOM | 2319 | CD | LYS | C3064 | 19.505 | -1.886 | 3.138 | 1.00 24.12 | С |
| ATOM | 2320 | CE | | C3064 | 19.616 | -0.407 | 3.519 | 1.00 24.30 | C |
| ATOM | 2321 | NZ | | C3064 | 18.388 | 0.060 | 4.209 | 1.00 24.43 | N |
| ATOM | 2322 | C | | C3064 | 24.519 | -2.408 | 3.281 | 1.00 24.84 | C |
| ATOM | 2323 | Ö | | C3064 | 25.132 | -1.401 | 2.939 | 1.00 24.90 | 0 |
| ATOM | 2324 | N | | C3065 | 24.916 | -3.166 | 4.297 | 1.00 26.22 | N |
| ATOM | 2325 | CA | | C3065 | 26.101 | -2.818 | 5.079 | 1.00 28.20 | С |
| ATOM | 2326 | CB | | C3065 | 26.184 | -3.693 | 6.324 | 1.00 28.57 | С |
| ATOM | 2327 | C | | C3065 | 27.396 | -2.943 | 4.277 | 1.00 30.15 | С |
| MOTA | 2328 | Ö | | C3065 | 28.346 | -2.188 | 4.492 | 1.00 29.72 | 0 |
| ATOM | 2329 | N | | C3066 | 27.435 | -3.903 | 3.361 | 1.00 32.11 | N |
| ATOM | 2330 | CA | | C3066 | 28.629 | -4.113 | 2.555 | 1.00 35.57 | c |
| ATOM | 2331 | CB | | C3066 | 28.706 | -5.577 | 2.115 | 1.00 36.03 | . С |
| ATOM | 2332 | CG | | C3066 | 30.087 | -5.993 | 1.635 | 1.00 38.01 | C |
| ATOM | 2333 | SD | | C3066 | 30.589 | -7.586 | 2.315 | 1.00 39.43 | S |
| ATOM | 2334 | CE | | C3066 | 29.820 | -8.664 | 1.141 | 1.00 38.43 | С |
| ATOM | 2335 | C | | C3066 | 28.641 | -3.186 | 1.340 | 1.00 37.25 | Č |
| ATOM | 2336 | 0 | | C3066 | 29.690 | -2.928 | 0.753 | 1.00 37.48 | Ō |
| ATOM | 2337 | N | | C3067 | 27.468 | -2.678 | 0.978 | 1.00 39.12 | N |
| ATOM | 2338 | CA | | C3067 | 27.372 | -1.782 | -0.158 | 1.00 41.84 | C |
| MOTA | 2339 | C | | C3067 | 27.338 | -2.554 | -1.458 | 1.00 43.68 | Č |
| ATOM | 2340 | Ö | | C3067 | 28.251 | -2.446 | -2.277 | 1.00 44.30 | ō |
| ATOM | 2341 | N | | C3068 | 26.281 | -3.337 | -1.648 | 1.00 45.16 | N |
| ATOM | 2342 | CA | | C3068 | 26.133 | -4.140 | -2.853 | 1.00 46.52 | C |
| ATOM | 2342 | CB | | C3068 | 27.012 | -5.409 | -2.771 | 1.00 46.98 | Č |
| ATOM | 2343 | | | C3068 | 26.723 | -6.268 | -3.880 | 1.00 47.83 | ō |
| ATOM | 2345 | | | C3068 | 26.756 | -6.154 | -1.469 | 1.00 47.19 | Ċ |
| | 2346 | C | | C3068 | 24.679 | | -3.076 | 1.00 47.27 | C |
| ATOM ATOM | 2347 | Ö | | C3068 | 23.940 | -4.800 | -2.123 | 1.00 47.53 | 0 |
| ATOM | 2348 | N | | C3069 | 24.272 | -4.597 | -4.341 | 1.00 47.97 | N |
| MOTA | 2349 | CA | | C3069 | 22.908 | -4.969 | -4.668 | 1.00 48.41 | Ċ |
| ATOM | 2350 | C | | C3069 | 22.848 | | -5.629 | 1.00 48.94 | Ċ |
| ATOM | 2351 | 0 | | C3069 | 22.349 | | -6.758 | 1.00 49.17 | Ō |
| ATOM | 2352 | | | C3069 | 23.304 | -7.244 | -5.257 | 1.00 49.26 | ő |
| TER | 2353 | OVI | | C3069 | 23,304 | , . 4.7.7 | 3.237 | 2.00 45.20 | Ŭ |
| ATOM | 2354 | С | | C3074 | 23 102 | -14.343 | -2.448 | 1.00 42.87 | С |
| | 2355 | 0 | | C3074 | | -14.155 | -1.552 | 1.00 42.07 | Õ |
| ATOM ATOM | 2356 | Ŋ | | C3074 | | -14.133 | -4.163 | 1.00 43.22 | N |
| ATOM | 2357 | CA | | C3074 | | -14.000 | -3.885 | 1.00 42.94 | C |
| ATOM | 2331 | CA | ابلای | C30/4 | 23.440 | -14.000 | -3.003 | 1.00 42.74 | Č |

| ATOM | 2358 | N | DUE | C3075 | | 21 902 | -14.845 | -2.228 | 1.00 | 12 92 | 1 | N |
|------|------|------|-----|-------|---|--------|---------|---------|------|-------|---|----|
| | | | | | | | | | | | | |
| MOTA | 2359 | CA | | C3075 | | | -15.212 | -0.890 | 1.00 | | | С |
| ATOM | 2360 | CB | | C3075 | | | -15.035 | -0.787 | | 43.13 | | С |
| ATOM | 2361 | CG | PHE | C3075 | | 19.484 | -13.638 | -0.400 | | 43.82 | | С |
| MOTA | 2362 | CD1 | PHE | C3075 | | 20.299 | -12.534 | -0.647 | 1.00 | 43.85 | (| С |
| ATOM | 2363 | CD2 | PHE | C3075 | | 18.243 | -13.429 | 0.199 | 1.00 | 43.74 | (| С |
| ATOM | 2364 | CE1 | PHE | C3075 | | 19.883 | -11.243 | -0.304 | 1.00 | 44.03 | | С |
| ATOM | 2365 | | | C3075 | | | -12.144 | 0.545 | | 44.13 | | C |
| ATOM | 2366 | CZ | | C3075 | | | -11.049 | 0.293 | | 44.14 | | č |
| ATOM | 2367 | C | | C3075 | | | -16.639 | -0.516 | | 42.74 | | c |
| ATOM | | | | | | | | | | | | |
| | 2368 | 0 | | C3075 | | | -17.007 | 0.661 | | 42.92 | | 0 |
| ATOM | 2369 | N | | C3076 | | | -17.438 | -1.518 | | 42.00 | | N |
| ATOM | 2370 | CA | | C3076 | | | -18.824 | -1.276 | | 41.00 | | С |
| MOTA | 2371 | CB | | C3076 | | | -19.615 | -2.587 | | 41.57 | | C |
| ATOM | 2372 | CG | GLN | C3076 | | | -19.865 | -3.119 | 1.00 | 42.06 | | С |
| MOTA | 2373 | CD | GLN | C3076 | | 20.286 | -20.695 | -2.171 | 1.00 | 42.45 | ı | C |
| ATOM | 2374 | OE1 | GLN | C3076 | | 19.056 | -20.670 | -2.243 | 1.00 | 42.81 | • | 0 |
| ATOM | 2375 | NE2 | GLN | C3076 | | 20.938 | -21.445 | -1.284 | 1.00 | 42.52 | 1 | N |
| MOTA | 2376 | С | | C3076 | | 23.892 | -18.977 | -0.584 | 1.00 | 40.27 | 1 | С |
| ATOM | 2377 | 0 | GLN | C3076 | | 24.216 | -20.060 | -0.103 | 1.00 | 40.25 | | 0 |
| ATOM | 2378 | N | | C3077 | | | -17.907 | -0.537 | | 38.81 | | N |
| ATOM | 2379 | CA | | C3077 | | | -17.981 | 0.148 | | 37.42 | | C |
| ATOM | 2380 | CB | | C3077 | | | -17.527 | -0.769 | | 39.03 | | C |
| | | | | | | | | | | | | C |
| ATOM | 2381 | CG | | C3077 | | | -16.075 | -1.152 | | 40.35 | | |
| ATOM | 2382 | | | C3077 | | | -15.635 | -1.514 | | 41.46 | | 0 |
| ATOM | 2383 | | | C3077 | | | -15.379 | -1.102 | | 40.89 | | 0 |
| MOTA | 2384 | С | | C3077 | | | -17.158 | 1.438 | | 35.34 | | С. |
| MOTA | 2385 | 0 | ASP | C3077 | | 26.916 | -16.556 | 1.848 | 1.00 | 35.66 | | 0 |
| MOTA | 2386 | N | LEU | C3078 | | 24.751 | -17.142 | 2.060 | 1.00 | 32.99 | | N |
| MOTA | 2387 | CA | LEU | C3078 | | 24.513 | -16.456 | 3.328 | 1.00 | 30.22 | | С |
| MOTA | 2388 | CB | LEU | C3078 | | 23.775 | -15.127 | 3.113 | 1.00 | 30.01 | | С |
| ATOM | 2389 | CG | LEU | C3078 | | 24.478 | -13.972 | , 2.393 | 1.00 | 30.35 | | C |
| ATOM | 2390 | CD1 | LEU | C3078 | | 23.555 | -12.762 | 2.352 | 1.00 | 29.89 | | С |
| ATOM | 2391 | | | C3078 | | | -13.615 | 3.114 | 1.00 | 31.03 | | С |
| MOTA | 2392 | С | | C3078 | | | -17.392 | 4.165 | | 27.99 | | Ċ |
| ATOM | 2393 | Õ | | C3078 | | | -17.927 | 3.659 | | 27.40 | | o |
| ATOM | 2394 | N | | C3079 | | | -17.589 | 5.435 | | 25.61 | | N |
| ATOM | 2395 | CA | | C3079 | | | -18.467 | 6.310 | | 24.01 | | Ċ |
| MOTA | 2396 | CB | | C3079 | • | | -19.876 | 6.284 | | 24.83 | | C |
| | | | | C3079 | | | | | | | | C |
| ATOM | 2397 | CG | | | | | -20.897 | 7.190 | | 25.45 | | |
| ATOM | 2398 | CD | | C3079 | • | | ~22.290 | 7.022 | | 26.01 | | C |
| ATOM | 2399 | | | C3079 | | | -23.022 | 6.110 | | 26.62 | | 0 |
| ATOM | 2400 | | | C3079 | | | -22.648 | 7.797 | | 25.76 | | 0 |
| ATOM | 2401 | С | | C3079 | | | -17.945 | 7.756 | | 22.32 | | С |
| MOTA | 2402 | 0 | | C3079 | | | -17.500 | 8.335 | | 21.78 | | 0 |
| MOTA | 2403 | N | VAL | C3080 | | 21.905 | -18.007 | 8.319 | 1.00 | 20.99 | | N |
| MOTA | 2404 | CA | VAL | C3080 | | 21.616 | -17554 | 9.685 | 1.00 | 19.93 | | С |
| MOTA | 2405 | CB | VAL | C3080 | | 20.634 | -16.347 | 9.666 | 1.00 | 19.55 | | С |
| ATOM | 2406 | CG1 | VAL | C3080 | | 20.302 | -15.911 | 11.099 | 1.00 | 18.41 | | С |
| ATOM | 2407 | .CG2 | VAL | C3080 | | 21.246 | -15.183 | 8.878 | 1.00 | 19.42 | | С |
| ATOM | 2408 | С | | C3080 | | | -18.667 | 10.550 | | 20.28 | | С |
| ATOM | 2409 | ō | | C3080 | | | -19.140 | 10.261 | | 19.70 | | ō |
| ATOM | 2410 | N | | C3081 | | | -19.075 | 11.606 | | 20.21 | | N |
| ATOM | 2411 | CA | | C3081 | | | -20.121 | 12.521 | | 21.05 | | C |
| ATOM | 2412 | CB | | C3081 | | | -21.290 | 12.559 | | 21.12 | | C |
| ATOM | | CB | | C3081 | | | -21.250 | 11.246 | | 20.96 | | C |
| ATOM | 2413 | | | C3081 | | | -23.067 | 11.542 | | 21.74 | | С |
| ATOM | 2414 | CDI | FEO | 03001 | | 23.033 | -23.007 | 11.042 | 1.00 | 21.74 | | ٠ |

| MOTA | 2415 | CD2 | LEU | C3081 | 21.497 | -22.498 | 10.489 | 1.00 | 20.34 | С |
|--------------|--------------|----------|-----|----------------|--------|--------------------|------------------|-------|----------------|--------|
| ATOM | 2416 | С | LEU | C3081 | 21.041 | -19.566 | 13.948 | 1.00 | 21.83 | С |
| ATOM | 2417 | 0 | LEU | C3081 | 21.340 | -18.399 | 14.211 | .1.00 | 20.95 | 0 |
| ATOM | 2418 | N | ASN | C3082 | 20.546 | -20.411 | 14.855 | 1.00 | 22.96 | N |
| ATOM | 2419 | CA | ASN | C3082 | 20.322 | -20.043 | 16.262 | 1.00 | 24.19 | С |
| ATOM | 2420 | CB | ASN | C3082 | 18.857 | -20.281 | 16.654 | 1.00 | 24.95 | С |
| ATOM | 2421 | CG | | C3082 | | -19.223 | 16.101 | | 25.21 | С |
| ATOM | 2422 | | | C3082 | | -18.100 | 16.611 | | 26.05 | 0 |
| ATOM | 2423 | | | C3082 | | -19.577 | 15.055 | | 24.39 | N |
| ATOM | 2424 | C | | C3082 | | -20.890 | 17.184 | | 24.76 | C |
| ATOM | 2425 | ō | | C3082 | | -22.114 | 17.034 | | 24.23 | O |
| ATOM | 2426 | N | | C3083 | | -20.258 | 18.133 | | 24.88 | N |
| ATOM | 2427 | CA | | C3083 | | -21.024 | 19.046 | | 26.41 | Ċ |
| ATOM | 2428 | CB | | C3083 | | -20.147 | 19.619 | | 26.57 | c |
| ATOM | 2429 | CG | | C3083 | | -19.088 | 20.603 | | 27.00 | Ċ |
| ATOM | 2430 | | | C3083 | | -18.255 | 21.047 | | 28.80 | · o |
| ATOM | 2431 | | | C3083 | | -19.115 | 20.952 | | 25.26 | N |
| ATOM | 2432 | C | | C3083 | | -21.676 | 20.159 | | 26.81 | c |
| ATOM | 2433 | 0 | | C3083 | | -21.536 | 20.178 | | 26.49 | ō |
| ATOM | 2434 | N | | C3084 | | -22.390 | 21.078 | | 27.91 | Ŋ |
| MOTA | 2435 | CA | | C3084 | | -23.070 | 22.132 | | 28.75 | C |
| ATOM | 2436 | CB | | C3084 | | -24.035 | 22.917 | | 29.93 | č |
| ATOM | 2430 | CG | | C3084 | | -23.506 | 23.335 | | 31.45 | ; c |
| ATOM | 2437 | CD | | C3084 | | -24.594 | 23.966 | | 32.85 | . c |
| ATOM | 2439 | | | C3084 | | -24.298 | 24.397 | | 33.48 | Ö |
| ATOM | 2440 | | | C3084 | | -25.752 | 24.029 | | 33.46 | Ö |
| ATOM | 2441 | C | | C3084 | | -23.732 | 23.092 | | 28.50 | c |
| ATOM | 2442 | 0 | | C3084 | | -22.169 | 23.714 | | 28.13 | 0 |
| ATOM | 2442 | N | | C3085 | | -20.917 | 23.215 | | 28.57 | N |
| ATOM | 2444 | | | C3085 | | -20.001 | 24.085 | | 28.82 | C |
| | | CA | | C3085 | | | | | 29.93 | c |
| MOTA MOTA | 2445 | CB | | C3085 | | -18.929 -19.469 | 24.670 | | 31.34 | C |
| | 2446 | CG CD | | C3085 | | | 25.692 | | 33.11 | c |
| ATOM | 2447 | NE | | C3085 | | -18.409 | 26.713 27.683 | | 33.67 | N N |
| ATOM | 2448 | | | C3085 | | -18.936 -19.217 | 27.398 | • | 34.16 | C |
| ATOM ATOM | 2449 | CZ | | C3085 | | -19.014 | 26.171 | | 34.21 | N |
| | 2450 | | | | | | | | | N |
| MOTA | 2451 | | | C3085 | | -19.715 | 28.330 | • | 33.81 | C |
| ATOM | 2452 | C | | C3085 | | -19.332 | 23.318 | | 28.44 | 0 |
| ATOM | 2453 | O N | | C3085 | | -18.667 -19.496 | 23.912 | | 28.67 27.15 | N |
| ATOM ATOM | 2454 | N CA | | C3086 C3086 | | | 21.996 21.170 | | 26.89 | C |
| ATOM | 2455 2456 | C | | C3086 | | -18.928 -17.712 | 20.316 | | 26.43 | C |
| | | | | | | | | | 26.94 | 0 |
| MOTA | 2457 | 0 | | C3086 C3087 | | -17.229 | 19.581 20.396 | | 25.34 | Ŋ |
| ATOM ATOM | 2458 2459 | N CA | | C3087 | | -17.218 -16.043 | 19.622 | | 25.00 | Č |
| | 2459 | CB | | C3087 | | | | | | C |
| ATOM | | | | C3087 | | -15.361 | 20.300 | | 25.01 24.71 | C |
| ATOM | 2461 | C | | C3087 | | -16:355 | 18.163 | | 23.78 | 0 |
| ATOM | 2462 | 0 | | | | -17.394 | 17.867 | | | • |
| ATOM | 2463 | N | | C3088 | | -15.457 | 17.231 | | 23.74 | N |
| ATOM | 2464 | CD | | C3088 C3088 | | -14.291 | 17.448 | | 24.91 23.12 | C C |
| ATOM | 2465 | CA | | | | -15.631 | 15.800 | | | c |
| ATOM ATOM | 2466 | CB | | C3088 | | -14.762 | 15.136 | | 24.34 | C |
| ATOM | 2467 2468 | CG | | C3088 | | -13.593 | 16.083 | | 24.53 | c |
| ATOM | 2468 | С О | | C3088 | | -15.157 -14.198 | 15.466 16.070 | | 22.17 21.42 | 0 |
| ATOM | 2469 | Ŋ | | C3089 | | -15.826 | 14.512 | | 20.38 | N |
| ATOM | 2470 | CA | | C3089 | | -15.469 | 14.098 | | 19.72 | C |
| OI OLI | 741I | CA | 111 | 03003 | 24.120 | 13.403 | 14.030 | 1.00 | 17.12 | C |

| ATOM | 2472 | CB | TYR | C3089 | 25.149 | -16.054 | 15.097 | 1.00 19.67 | С |
|--------------|--------------|----------|-----|----------------|--------|--------------------|----------------|--------------------------|--------|
| ATOM | 2473 | CG | TYR | C3089 | 25.352 | -17.564 | 15.029 | 1.00 19.93 | С |
| ATOM | 2474 | CD1 | TYR | C3089 | 26.410 | -18.110 | 14.294 | 1.00 21.07 | C |
| MOTA | 2475 | CE1 | TYR | C3089 | 26.594 | -19.497 | 14.194 | 1.00 20.45 | С |
| MOTA | 2476 | CD2 | TYR | C3089 | 24.477 | -18.446 | 15.672 | 1.00 20.53 | С |
| ATOM | 2477 | CE2 | TYR | C3089 | 24.653 | -19.848 | 15.578 | 1.00 20.54 | С |
| ATOM | 2478 | CZ | TYR | C3089 | 25.717 | -20.359 | 14.833 | 1.00 20.66 | С |
| MOTA | 2479 | OH | TYR | C3089 | 25.908 | -21.725 | 14.713 | 1.00 19.20 | 0 |
| MOTA | 2480 | С | TYR | C3089 | 24.428 | -15.972 | 12.671 | 1.00 19.17 | С |
| MOTA | 2481 | 0 | TYR | C3089 | 23.820 | -16.944 | 12.213 | 1.00 17.72 | 0 |
| MOTA | 2482 | N | PHE | C3090 | 25.340 | -15.295 | 11.967 | 1.00 19.73 | N |
| MOTA | 2483 | CA | PHE | C3090 | 25.729 | -15.704 | 10.607 | 1.00 20.26 | С |
| MOTA | 2484 | CB | PHE | C3090 | 26.310 | -14.529 | 9.800 | 1.00 20.96 | С |
| ATOM | 2485 | CG | PHE | C3090 | | -13.607 | 9.198 | 1.00 20.15 | С |
| MOTA | 2486 | CD1 | PHE | C3090 | 24.812 | -12.499 | 9.902 | 1.00 20.78 | С |
| MOTA | 2487 | | | C3090 | 24.791 | -13.831 | 7.912 | 1.00 20.37 | С |
| MOTA | 2488 | CE1 | PHE | C3090 | 23.880 | -11.620 | 9.330 | 1.00 20.73 | С |
| ATOM | 2489 | CE2 | | C3090 | | -12.964 | 7.326 | 1.00 20.67 | С |
| ATOM | 2490 | CZ | | C3090 | 23.404 | -11.853 | 8.040 | 1.00 20.35 | С |
| ATOM | 2491 | С | PHE | C3090 | | -16.812 | 10.637 | 1.00 20.91 | С |
| ATOM | 2492 | 0 | | C3090 | | -16.598 | 11.117 | 1.00 20.54 | 0 |
| ATOM | 2493 | N | | C3091 | | -17.986 | 10.116 | 1.00 21.82 | N |
| MOTA | 2494 | CA | | C3091 | | -19.113 | 10.073 | 1.00 22.73 | C |
| MOTA | 2495 | CB | | C3091 | - | -20.435 | 10.290 | 1.00 22.96 | C |
| MOTA | 2496 | OG | | C3091 | | -20.617 | 9.318 | 1.00 23.28 | 0 |
| MOTA | 2497 | С | | C3091 | | -19.164 | 8.738 | 1.00 23.33 | C |
| ATOM | 2498 | 0 | | C3091 | | -19.904 | 8.604 | 1.00 22.86 | 0 |
| ATOM | 2499 | N | | C3092 | 27.683 | | 7.762 | 1.00 23.62 | N |
| ATOM | 2500 | CA | | C3092 | | -18.319 | 6.436 | 1.00 24.85 | C |
| ATOM | 2501 | CB | | C3092 | | -19.439 | 5.558 | 1.00 25.88 | C |
| MOTA | 2502 | CG | | C3092 | | -19.357 | 4.064 | 1.00 28.11 | C |
| ATOM | 2503 | CD | | C3092 | | -19.339 | 3.762 | 1.00 29.40 | C |
| MOTA | 2504 | | | C3092 | | -20.131 | 4.310 | 1.00 31.43 | 0 |
| MOTA | 2505 | | | C3092 | | -18.441 | 2.874 | 1.00 30.15 | N |
| ATOM | 2506 | С | | C3092 | | -16.944 | 5.764 | 1.00 24.73 | С |
| ATOM | 2507 | 0 | | C3092 | | -16.472 | 5.637 | 1.00 24.71 | 0 |
| ATOM | 2508 | N | | C3093 | | -16.310 | 5.343 | 1.00 23.94 | N C |
| MOTA | 2509 | CA | | C3093 | | -14.994 | 4.685 | 1.00 23.97 1.00 23.95 | c |
| ATOM | 2510 | CB | | C3093 | | -13.909 | 5.706 | 1.00 23.83 | c |
| ATOM | 2511 | С | | C3093 | | -14.618 | 4.009 4.472 | 1.00 23.82 | 0 |
| MOTA | 2512 | O M | | C3093 C3094 | | -15.008 -13.841 | 2.910 | 1.00 23.02 | N |
| ATOM | 2513 | N CD | | C3094 | | -13.410 | 2.203 | 1.00 24.15 | Č |
| ATOM | 2514 | | | C3094 | | -13.414 | 2.177 | 1.00 24.13 | Č |
| ATOM | 2515 2516 | CA CB | | C3094 | | -13.414 | 0.801 | 1.00 24.26 | c |
| ATOM | 2517 | | | C3094. | | -12.461 | 1.144 | 1.00 24.20 | č |
| MOTA MOTA | 2518 | CG C | | C3094. | | -12.231 | 2.840 | 1.00 24.92 | Č |
| ATOM | 2519 | 0 | | C3094 | | -11.165 | 2.239 | 1.00 24.52 | ő |
| ATOM | 2520 | N | | C3095 | | -12.437 | 4.076 | 1.00 25.08 | N |
| ATOM | 2521 | CA | | C3095 | | -11.410 | 4.864 | 1.00 25.37 | C |
| ATOM | 2522 | CB | | C3095 | | -10.502 | 5.521 | 1.00 24.79 | C |
| ATOM | 2523 | CG | | C3095 | 33.015 | | 6.356 | 1.00 24.93 | Č |
| ATOM | 2524 | | | C3095 | 33.652 | | 5.760 | 1.00 24.60 | Č |
| MOTA | 2525 | | | C3095 | 32.883 | | 7.741 | 1.00 24.43 | C |
| ATOM | 2526 | | | C3095 | 34.148 | | 6.536 | 1.00 24.72 | C |
| ATOM | 2527 | | | C3095 | 33.374 | | 8.527 | 1.00 24.22 | · C |
| ATOM | 2528 | CZ | | C3095 | 34.008 | | 7.921 | 1.00 24.70 | С |
| | | | | | | | | | |

| ATOM | 2529 | С | PHE | C3095 | 34.288 | -12.163 | 5.928 | 1.00 25.61 | С |
|--------|------|-----|-----|-------|---------|---------|--------|------------|-----|
| ATOM | 2530 | 0 | PHE | C3095 | 33.766 | -13.101 | 6.537 | 1.00 26.06 | 0 |
| ATOM | 2531 | N | SER | C3096 | 35.538 | -11.773 | 6.164 | 1.00 26.42 | N |
| ATOM | 2532 | CA | SER | C3096 | 36.343 | -12.485 | 7.158 | 1.00 27.23 | С |
| MOTA | 2533 | CB | SER | C3096 | 37.709 | -12.857 | 6.558 | 1.00 27.32 | C |
| ATOM | 2534 | OG | | C3096 | | -11.725 | 6.054 | 1.00 28.68 | 0 |
| ATOM | 2535 | C | | C3096 | | -11.795 | 8.515 | 1.00 27.58 | С |
| MOTA | 2536 | 0 | | C3096 | | -12.259 | 9.349 | 1.00 28.21 | Ō |
| ATOM | 2537 | N | | C3097 | | -10.700 | 8.745 | 1.00 27.18 | N |
| ATOM | 2538 | CA | | C3097 | | -10.003 | 10.021 | 1.00 26.33 | C |
| MOTA | 2539 | C | | C3097 | | -10.462 | 10.971 | 1.00 26.17 | Č |
| | | | | | | | 10.845 | 1.00 25.72 | 0 |
| MOTA | 2540 | 0 | | C3097 | 34.322 | -11.584 | | 1.00 25.72 | N |
| MOTA | 2541 | N | | C3098 | | -9.610 | 11.916 | 1.00 23.23 | C |
| ATOM | 2542 | CA | | C3098 | 33.347 | -9.971 | 12.864 | | |
| ATOM | 2543 | CB | | C3098 | 33.759 | -9.591 | 14.289 | 1.00 25.96 | C |
| ATOM | 2544 | CG | | C3098 | | -10.259 | 14.723 | 1.00 28.19 | С |
| ATOM | 2545 | CD | | C3098 | | -10.576 | 16.208 | 1.00 29.56 | C |
| MOTA | 2546 | CE | | C3098 | 35.022 | -9.324 | 17.053 | 1.00 30.68 | С |
| ATOM . | 2547 | NZ | | C3098 | 35.150 | -9.647 | 18.505 | 1.00 32.82 | N |
| ATOM | 2548 | С | | C3098 | 32.013 | -9.313 | 12.498 | 1.00 22.87 | С |
| MOTA | 2549 | 0 | LYS | C3098 | 31.984 | -8.155 | 12.082 | 1.00 22.97 | 0 |
| ATOM | 2550 | И | ILE | C3099 | 30.919 | -10.060 | 12.659 | 1.00 21.29 | N |
| MOTA | 2551 | CA | ILE | C3099 | ,29.567 | -9.589 | 12.316 | 1.00 19.46 | С |
| MOTA | 2552 | CB | ILE | C3099 | 28.918 | -10.546 | 11.251 | 1.00 19.44 | C |
| MOTA | 2553 | CG2 | ILE | C3099 | 27.577 | -9.987 | 10.769 | 1.00 18.38 | С |
| MOTA | 2554 | CG1 | ILE | C3099 | 29.869 | -10.742 | 10.062 | 1.00 19.30 | С |
| ATOM | 2555 | CD1 | ILE | C3099 | 29.447 | -11.853 | 9.103 | 1.00 19.40 | С |
| ATOM | 2556 | C | | C3099 | 28.632 | -9.537 | 13.544 | 1.00 18.29 | C |
| ATOM | 2557 | 0 | | C3099 | | -10.568 | 14.165 | 1.00 18.68 | 0 |
| ATOM | 2558 | N | | C3100 | 28.109 | -8.357 | 13.888 | 1.00 16.88 | N |
| ATOM | 2559 | CA | | C3100 | 27.195 | -8.233 | 15.036 | 1.00 15.59 | С |
| ATOM | 2560 | CB | | C3100 | 27.643 | -7.078 | 15.956 | 1.00 15.65 | c |
| ATOM | 2561 | CG | | C3100 | 29.076 | -7.231 | 16.505 | 1.00 15.70 | Č |
| ATOM | 2562 | | | C3100 | 29.492 | -8.034 | 17.626 | 1.00 15.13 | č |
| ATOM | 2563 | | | C3100 | 30.901 | -7.910 | 17.735 | 1.00 15.15 | c |
| | | CE3 | | C3100 | 28.813 | -8.846 | 18.547 | 1.00 15.20 | c |
| ATOM | 2564 | | | C3100 | 30.220 | -6.668 | 15.997 | 1.00 15.40 | C |
| ATOM | 2565 | | | | | | | | N |
| ATOM | 2566 | | | C3100 | 31.321 | -7.074 | 16.734 | 1.00 15.83 | |
| MOTA | 2567 | | | C3100 | 31.639 | -8.570 | 18.730 | 1.00 15.21 | C |
| ATOM | 2568 | | | C3100 | 29.549 | -9.504 | 19.538 | 1.00 15.48 | . C |
| ATOM | 2569 | | | C3100 | 30.950 | -9.358 | 19.618 | 1.00 15.73 | C |
| MOTA | 2570 | C | | C3100 | 25.746 | -8.022 | 14.533 | 1.00 15.44 | C |
| ATOM | 2571 | 0 | | C3100 | 25.438 | -6.991 | 13.924 | 1.00 14.84 | 0 |
| ATOM | 2572 | N | | C3101 | 24.875 | -9.003 | 14.800 | 1.00 14.06 | N |
| ATOM | 2573 | CA | LEU | C3101 | 23.469 | -9.004 | 14.348 | 1.00 13.05 | C |
| ATOM | 2574 | CB | | C3101 | | -10.161 | 13.357 | 1.00 13.07 | C |
| ATOM | 2575 | CG | | C3101 | | -10.623 | 13.084 | 1.00 12.96 | C |
| MOTA | 2576 | | | C3101 | 21.208 | | 12.015 | 1.00 13.42 | C |
| ATOM | 2577 | CD2 | | C3101 | | -12.083 | 12.624 | 1.00 14.82 | С |
| MOTA | 2578 | С | LEU | C3101 | 22.382 | -9.133 | 15.430 | 1.00 12.57 | C |
| MOTA | 2579 | 0 | | C3101 | 22.597 | | 16.450 | 1.00 11.63 | 0 |
| MOTA | 2580 | N | SER | C3102 | 21.215 | -8.525 | 15.181 | 1.00 12.95 | N |
| ATOM | 2581 | CA | SER | C3102 | 20.054 | -8.615 | 16.092 | 1.00 13.03 | С |
| ATOM | 2582 | CB | SER | C3102 | 20.128 | -7.536 | 17.187 | 1.00 13.35 | С |
| ATOM | 2583 | OG | SER | C3102 | 19.148 | -7.749 | 18.205 | 1.00 12.78 | . 0 |
| ATOM | 2584 | С | | C3102 | 18.736 | | 15.297 | 1.00 13.43 | C |
| ATOM | 2585 | 0 | | C3102 | 18.687 | | 14.298 | 1.00 13.38 | 0 |
| - | - " | | | _ | | | - | | _ |

| MOTA | 2586 | N | ILE | C3103 | 17.687 | -9.197 | 15.741 | 1.00 13.23 | N |
|------|------|-----|-----|-------|----------------|---------|--------|--------------------------|---|
| MOTA | 2587 | CA | ILE | C3103 | 16.355 | -9.215 | 15.082 | 1.00 14.65 | С |
| MOTA | 2588 | CB | ILE | C3103 | 16.135 | -10.552 | 14.290 | 1.00 15.02 | C |
| MOTA | 2589 | CG2 | ILE | C3103 | 14.776 | -10.534 | 13.581 | 1.00 14.81 | С |
| MOTA | 2590 | CG1 | ILE | C3103 | 17.254 | -10.764 | 13.267 | 1,00 15.40 | С |
| ATOM | 2591 | CD1 | ILE | C3103 | 17.113 | -12.053 | 12.443 | 1.00 16.79 | C |
| ATOM | 2592 | C | | C3103 | 15.180 | -9.123 | 16.087 | 1.00 15.28 | С |
| ATOM | 2593 | 0 | | C3103 | 15.239 | -9.717 | 17.166 | 1.00 15.06 | Ō |
| ATOM | 2594 | N | | C3104 | 14.109 | -8.414 | 15.726 | 1.00 16.55 | N |
| ATOM | 2595 | CA | | C3104 | 12.930 | -8.295 | 16.614 | 1.00 17.82 | C |
| ATOM | 2596 | СВ | | C3104 | 13.077 | -7.067 | 17.527 | 1.00 18.38 | Č |
| ATOM | 2597 | OG | | C3104 | 12.058 | -7.028 | 18.524 | 1.00 18.13 | 0 |
| ATOM | 2598 | C | | C3104 | 11.629 | -8.186 | 15.793 | 1.00 19.18 | c |
| ATOM | 2599 | ō | | C3104 | 11.672 | -7.850 | 14.608 | 1.00 18.60 | 0 |
| MOTA | 2600 | N | | C3105 | 10.475 | -8.466 | 16.405 | 1.00 21.28 | N |
| ATOM | 2601 | CA | | C3105 | 9.209 | | 15.660 | 1.00 23.07 | C |
| MOTA | 2602 | CB | | C3105 | 8.964 | -9.664 | 14.877 | 1.00 24.36 | č |
| ATOM | 2603 | CG | | C3105 | | -10.856 | 15.749 | 1.00 25.51 | c |
| ATOM | 2604 | | | C3105 | | -11.219 | 16.474 | 1.00 26.93 | č |
| ATOM | 2605 | | | C3105 | | -11.815 | 15.986 | 1.00 26.74 | N |
| ATOM | 2606 | | | C3105 | | -12.721 | 16.820 | 1.00 27.20 | C |
| ATOM | 2607 | | | C3105 | | -12.383 | 17.132 | 1.00 27.20 | Ŋ |
| | | | | | 7.927 | -8.081 | 16.452 | 1.00 24.09 | C |
| ATOM | 2608 | C | | C3105 | | | | | 0 |
| ATOM | 2609 | 0 | | C3105 | 7.913 6.851 | -8.058 | 17.686 | 1.00 23.14 1.00 25.15 | N |
| ATOM | 2610 | N | | C3106 | | -7.870 | 15.692 | | C |
| MOTA | 2611 | CA | | C3106 | 5.506 | -7.616 | 16.212 | 1.00 26.55 | |
| ATOM | 2612 | CB | | C3106 | 5.100 | | 16.097 | 1.00 26.80 | С |
| ATOM | 2613 | | | C3106 | 5.097 | | 14.717 | 1.00 27.05 | 0 |
| ATOM | 2614 | | | C3106 | 6,052 | -5.258 | 16.880 | 1.00 27.26 | C |
| ATOM | 2615 | С | | C3106 | 4.549 | | 15.339 | 1.00 27.26 | С |
| ATOM | 2616 | 0 | | C3106 | 4.987 | | 14.477 | 1.00 26.93 | 0 |
| ATOM | 2617 | N | | C3107 | 3.245 | -8.287 | 15.539 | 1.00 28.56 | N |
| ATOM | 2618 | CA | | C3107 | | ~9.067 | 14.732 | 1.00 30.14 | C |
| ATOM | 2619 | CB | | C3107 | 0.977 | -9.243 | 15.474 | 1.00 32.49 | С |
| MOTA | 2620 | CG | | C3107 | 0.498 | -7.968 | 16.133 | 1.00 34.70 | C |
| ATOM | 2621 | | | C3107 | 0.406 | | 15.440 | 1.00 37.09 | 0 |
| MOTA | 2622 | | | C3107 | 0.209 | | 17.348 | 1.00 36.52 | 0 |
| MOTA | 2623 | C | | C3107 | 2.065 | | 13.334 | 1.00 29.74 | C |
| ATOM | 2624 | 0 | | C3107 | 1.264 | | 12.575 | 1.00 30.83 | 0 |
| ATOM | 2625 | N | | C3108 | 2.762 | | 12.979 | 1.00 28.55 | N |
| ATOM | 2626 | CA | | C3108 | 2.578 | | 11.665 | 1.00 27.66 | C |
| ATOM | 2627 | CB | | C3108 | 1.942 | | 11.822 | 1.00 27.82 | C |
| ATOM | 2628 | CG | | C3108 | 0.557 | | 12.466 | 1.00 28.58 | C |
| MOTA | 2629 | CD | | C3108 | 0.012 | | 12.681 | 0.05 28.18 | C |
| ATOM | 2630 | | | C3108 | -1.083 | | 13.214 | 0.05 28.21 | 0 |
| ATOM | 2631 | | | C3108 | 0.779 | | | | N |
| ATOM | 2632 | C | | C3108 | 3.845 | | 10.812 | 1.00 26.77 | C |
| MOTA | 2633 | 0 | | C3108 | 3.760 | | 9.582 | 1.00 25.82 | 0 |
| ATOM | 2634 | N | | C3109 | 5.015 | | 11.449 | 1.00 25.68 | N |
| MOTA | 2635 | CA | | C3109 | 6.268 | | 10.697 | 1.00 24.08 | C |
| MOTA | 2636 | CB | | C3109 | 6.441 | | 10.221 | 1.00 25.01 | c |
| ATOM | 2637 | CG | | C3109 | 6.572 | | 11.343 | 1.00 26.02 | C |
| MOTA | 2638 | | | C3109 | 7.763 | | 12.062 | 1.00 26.89 | C |
| MOTA | 2639 | | | C3109 | 5.505 | | 11.682 | 1:00 26.71 | C |
| MOTA | 2640 | | | C3109 | 7.889 | | 13.105 | 1.00 27.26 | C |
| MOTA | 2641 | | | C3109 | 5.616 | | 12.725 | 1.00 27.81 | C |
| ATOM | 2642 | CZ | PHE | C3109 | 6.811 | -2.156 | 13.437 | 1.00 27.24 | C |

| ATOM | 2643 | С | PHE | C3109 | 7.497 | -6.950 | 11.497 | 1.00 22.66 | C |
|--------------|--------------|-----------|-----|-------|------------------|------------------|------------------|--------------------------|-----|
| ATOM | 2644 | 0 | PHE | C3109 | 7.382 | -7.267 | 12.681 | 1.00 21.87 | 0 |
| MOTA | 2645 | N | VAL | C3110 | 8.658 | -6.992 | 10.833 | 1.00 20.94 | N |
| ATOM | 2646 | CA | VAL | C3110 | 9.932 | -7.396 | 11.460 | 1.00 19.58 | С |
| ATOM | 2647 | CB | VAL | C3110 | 10.402 | -8.790 | 10.931 | 1.00 20.14 | С |
| MOTA | 2648 | CG1 | VAL | C3110 | 10.731 | -8.705 | 9.443 | 1.00 20.40 | С |
| ATOM | 2649 | CG2 | VAL | C3110 | 11.639 | -9.268 | 11.707 | 1.00 21.57 | С |
| ATOM | 2650 | С | VAL | C3110 | 11.049 | -6.374 | 11.162 | 1.00 18.29 | С |
| ATOM | 2651 | 0 | | C3110 | 10.982 | -5.675 | 10.154 | 1.00 16.70 | 0 |
| ATOM | 2652 | N | | C3111 | 12.065 | -6.298 | 12.035 | 1.00 17.21 | N |
| ATOM | 2653 | CA | | C3111 | 13.210 | -5.383 | 11.852 | 1.00 16.21 | С |
| MOTA | 2654 | CB | | C3111 | 13.109 | -4.122 | 12.781 | 1.00 16.74 | С |
| ATOM | 2655 | OG1 | | C3111 | 13.100 | -4.528 | 14.159 | 1.00 19.56 | 0 |
| MOTA | 2656 | | | C3111 | 11.851 | -3.321 | 12.485 | 1.00 18.23 | С |
| ATOM | 2657 | C | | C3111 | 14.551 | -6.096 | 12.159 | 1.00 15.10 | С |
| ATOM | 2658 | 0 | | C3111 | 14.575 | -7.053 | 12.945 | 1.00 13.98 | 0 |
| ATOM | 2659 | N | | C3112 | 15.643 | -5.638 | 11.532 | 1.00 13.72 | Ŋ |
| MOTA | 2660 | CA | | C3112 | 16.996 | -6.210 | 11.737 | 1.00 14.06 | C |
| ATOM | 2661 | CB | | C3112 | 17.266 | -7.324 | 10.712 | 1.00 13.98 | Ċ |
| ATOM | 2662 | C | | C3112 | 18.092 | -5.135 | 11.630 | 1.00 13.79 | Ċ |
| ATOM | 2663 | 0 | | C3112 | 17.936 | -4.164 | 10.884 | 1.00 14.41 | ō |
| ATOM | 2664 | N | | C3113 | 19.194 | -5.320 | 12.364 | 1.00 13.18 | N |
| ATOM | 2665 | CA | | C3113 | 20.321 | -4.369 | 12.395 | 1.00 12.99 | c |
| ATOM | 2666 | CB | | C3113 | 20.321 | -3.510 | 13.665 | 1.00 12.53 | č |
| ATOM | 2667 | OG | | C3113 | 21.209 | -2.499 | 13.724 | 1.00 12.04 | Ö |
| ATOM | 2668 | C | | C3113 | 21.690 | -5.103 | 12.369 | 1.00 13.25 | č |
| ATOM | 2669 | o | | C3113 | 21.875 | -6.075 | 13.097 | 1.00 13.23 | ō |
| ATOM | 2670 | N | | C3114 | 22.636 | -4.611 | 11.555 | 1.00 12.44 | N |
| ATOM | 2671 | CA | | C3114 | 23.972 | -5.230 | 11.374 | 1.00 13.03 | Ċ |
| ATOM | 2672 | CB | | C3114 | 24.030 | -5.984 | 9.989 | 1.00 13.14 | c |
| ATOM | 2673 | | | C3114 | 25.467 | -6.425 | 9.641 | 1.00 12.50 | c |
| ATOM | 2674 | | | C3114 | 23.117 | -7.194 | 10.016 | 1.00 13.33 | Ċ |
| ATOM | 2675 | CGZ | | C3114 | 25.161 | -4.248 | 11.419 | 1.00 13.11 | C |
| ATOM | 2676 | Ö | | C3114 | 25.101 | -3.171 | 10.834 | 1.00 11.64 | Ö |
| ATOM | 2677 | N | | C3115 | 26.245 | -4.631 | 12.101 | 1.00 11.04 | N |
| ATOM | 2678 | CA | | C3115 | 27.463 | -3.797 | 12.176 | 1.00 14.05 | Č |
| ATOM | 2679 | CB | | C3115 | 27.717 | -3.208 | 13.593 | 1.00 15.10 | c |
| ATOM | 2680 | | | C3115 | 28.902 | -2.217 | 13.532 | 1.00 16.68 | Č |
| ATOM | 2681 | | | C3115 | 26.482 | -2.477 | 14.122 | 1.00 15.85 | C |
| ATOM | 2682 | | | C3115 | 26.657 | -1.949 | 15.549 | 1.00 15.56 | č |
| ATOM | 2683 | CDI | | C3115 | 28.699 | -4.655 | 11.836 | 1.00 16.02 | Č |
| ATOM | 2684 | 0 | | C3115 | 28.900 | -5.714 | 12.444 | 1.00 14.67 | Ö |
| ATOM | 2685 | N | | C3116 | 29.519 | -4.195 | 10.883 | 1.00 14.07 | N |
| ATOM | 2686 | | | C3116 | 30.741 | -4.920 | 10.469 | 1.00 10.42 | C |
| MOTA | 2687 | CA CB | | C3116 | 30.864 | -4.910 | 8.939 | 1.00 17.73 | č |
| | | | | | | | 8.157 | | C |
| ATOM | 2688 | CG CD1 | | C3116 | 29.646 29.914 | -5.423 -5.349 | 6.660 | 1.00 17.27 1.00 17.70 | C |
| ATOM ATOM | 2689 2690 | | | C3116 | 29.339 | -6.855 | 8.570 | 1.00 17.70 | · C |
| MOTA | 2691 | CDZ | | C3116 | 32.016 | -4.322 | 11.099 | 1.00 18.48 | Č |
| ATOM | 2692 | 0 | | C3116 | 32.185 | -3.101 | 11.134 | 1.00 16.07 | 0 |
| | | | | C3117 | | | | | N |
| ATOM ATOM | 2693 2694 | N CA | | C3117 | 32.926 34.150 | -5.184 -4.718 | 11.562 12.227 | 1.00 20.56 1.00 23.53 | C |
| | 2694 2695 | CA | | C3117 | 33.939 | -4.718 -4.757 | 13.754 | 1.00 23.53 | C |
| ATOM | | CB | | C3117 | | -4.757 -4.587 | | 1.00 24.06 | C |
| ATOM | 2696 | CG | | | 35.200 | | 14.608 | | c |
| ATOM | 2697 | CD OF1 | | C3117 | 34.952 | -4.835 -5.946 | 16.103 16.473 | 1.00 25.52 1.00 25.65 | 0 |
| MOTA | 2698 | | | C3117 | 34.507 | -5.946 -3.917 | | 1.00 25.88 | 0 |
| MOTA | 2699 | OEZ | GLU | COTTI | 35.203 | -3.911 | 16.913 | 1.00 73.88 | U |

| MOTA | 2700 | С | GLU | C3117 | 35.429 | -5.488 | 11.878 | 1.00 25.38 | С |
|------|------|-----|-----|-------|--------|---------------------|--------|------------|---|
| ATOM | 2701 | 0 | GLU | C3117 | 35.403 | -6.695 | ì1.654 | 1.00 25.28 | 0 |
| MOTA | 2702 | N | GLU | C3118 | 36.545 | -4.766 | 11.840 | 1.00 28.60 | N |
| ATOM | 2703 | CA | | C3118 | 37.857 | -5.346 | 11.559 | 1.00 32.23 | C |
| ATOM | 2704 | CB | | C3118 | 38.321 | -4.996 | 10.139 | 1.00 33.43 | Ċ |
| ATOM | 2705 | CG | | C3118 | 37.520 | -5.678 | 9.038 | 1.00 35.47 | č |
| ATOM | 2706 | CD | | C3118 | 38.123 | -5.482 | 7.657 | 1.00 36.73 | Č |
| ATOM | 2707 | | | C3118 | 37.561 | -6.029 | 6.683 | 1.00 37.62 | 0 |
| ATOM | 2708 | | | C3118 | 39.156 | -4.786 | 7.540 | 1.00 37.51 | 0 |
| ATOM | 2709 | C | | C3118 | 38.857 | -4.800 | 12.576 | 1.00 37.31 | C |
| | | | | C3118 | | | | 1.00 33.91 | |
| ATOM | 2710 | 0 | | | 39.168 | -3.608 | 12.576 | | 0 |
| ATOM | 2711 | N | | C3119 | 39.348 | -5.678 | 13.444 | 1.00 36.07 | N |
| ATOM | 2712 | CA | | C3119 | 40.308 | -5.298 | 14.477 | 1.00 37.92 | C |
| ATOM | 2713 | CB | | C3119 | 40.307 | -6.343 | 15.597 | 1.00 38.97 | C |
| MOTA | 2714 | CG | | C3119 | 38.908 | -6.622 | 16.137 | 1.00 39.98 | С |
| MOTA | 2715 | | | C3119 | 38.271 | -5.753 | 16.737 | 1.00 40.51 | 0 |
| ATOM | 2716 | | | C3119 | 38.424 | -7.841 | 15.919 | 1.00 40.65 | N |
| MOTA | 2717 | С | | C3119 | 41.713 | -5.169 | 13.889 | 1.00 38.71 | C |
| ATOM | 2718 | 0 | | C3119 | 41.850 | -5.354 | 12.662 | 1.00 39.38 | 0 |
| ATOM | 2719 | OXT | ASN | C3119 | 42.661 | -4.885 | 14.657 | 1.00 39.94 | 0 |
| TER | 2720 | | ASN | C3119 | | | | | |
| MOTA | 2721 | 0 | HOH | W5001 | 1.203 | 5.537 | 8.026 | 1.00 17.73 | 0 |
| ATOM | 2722 | 0 | HOH | W5002 | 14.815 | 9.909 | 2.322 | 1.00 14.32 | 0 |
| ATOM | 2723 | 0 | нон | W5003 | 23.904 | 8.622 | 37.957 | 1.00 27.02 | 0 |
| MOTA | 2724 | 0 | HOH | W5004 | 20.469 | 3.444 | 3.735 | 1.00 17.55 | 0 |
| ATOM | 2725 | 0 | нон | W5005 | 24.018 | 4.203 | 28.855 | 1.00 20.10 | 0 |
| ATOM | 2726 | 0 | | W5006 | 10.973 | 5.376 | 28.684 | 1.00 19.79 | 0 |
| ATOM | 2727 | 0 | | W5007 | 22.784 | 15.314 | 34.546 | 1.00 22.90 | 0 |
| ATOM | 2728 | 0 | | W5008 | 23.453 | 4.929 | 3.777 | 1.00 19.63 | 0 |
| ATOM | 2729 | Ö | | W5009 | 23.062 | 1.129 | 4.843 | 1.00 21.68 | Ō |
| ATOM | 2730 | ō | | W5010 | 25.642 | 18.163 | 37.608 | 1.00 19.94 | Ö |
| ATOM | 2731 | Ō | | W5011 | 23.184 | 2.653 | 2.606 | 1.00 26.65 | Ō |
| ATOM | 2732 | Ö | | W5012 | 28.019 | 0.947 | 5.252 | 1.00 22.66 | Ö |
| ATOM | 2733 | 0 | | W5013 | 4.711 | 21.958 | 2.912 | 1.00 24.85 | Ö |
| ATOM | 2734 | 0 | | W5014 | 36.483 | 3.458 | 10.706 | 1.00 31.97 | Ö |
| ATOM | 2735 | 0 | | W5015 | 17.241 | 0.177 | 14.610 | 1.00 23.93 | Ö |
| ATOM | 2736 | Ö | | W5016 | | -15.296 | 11.672 | 1.00 22.95 | ő |
| ATOM | 2737 | 0 | | W5017 | 19.479 | 14.186 | -2.520 | 1.00 25.49 | Ö |
| ATOM | 2738 | 0 | | W5017 | 27.283 | 10.084 | 6.422 | 1.00 23.49 | 0 |
| ATOM | 2739 | Ö | | W5019 | 14.135 | 8.932 | 34.920 | 1.00 24.49 | 0 |
| ATOM | 2740 | Ö | | W5020 | 36.044 | 2.408 | 16.583 | 1.00 20.55 | 0 |
| ATOM | 2741 | Ö | | W5023 | | -17.363 | 3.678 | 1.00 32.30 | 0 |
| ATOM | 2742 | o | | W5021 | 15.667 | -0.884 | 2.725 | 1.00 19.73 | 0 |
| ATOM | 2743 | 0 | | W5022 | 9.740 | -0.876 | 42.696 | 1.00 31.93 | 0 |
| | 2744 | | | W5023 | | -24.311 | | | 0 |
| ATOM | | 0 | | | | | 26.736 | 1.00 36.28 | |
| ATOM | 2745 | 0 | | W5025 | 16.170 | 2.461 | 13.853 | 1.00 22.79 | 0 |
| ATOM | 2746 | 0 | | W5026 | 13.623 | -1. 9 72 | 15.922 | 1.00 33.10 | 0 |
| ATOM | 2747 | 0 | | W5027 | 35.568 | -7.137 | 18.918 | 1.00 28.33 | 0 |
| ATOM | 2748 | 0 | | W5028 | 21.193 | 8.337 | 22.471 | 1.00 24.39 | 0 |
| ATOM | 2749 | 0 | | W5029 | 0.905 | 8.530 | 3.669 | 1.00 29.99 | 0 |
| ATOM | 2750 | 0 | | W5030 | 26.791 | 21.664 | 30.504 | 1.00 26.91 | 0 |
| ATOM | 2751 | 0 | | W5031 | 12.687 | -4.279 | 3.191 | 1.00 33.49 | 0 |
| ATOM | 2752 | 0 | | W5032 | 25.981 | 5.485 | 38.408 | 1.00 30.01 | 0 |
| ATOM | 2753 | 0 | | W5033 | | -22.326 | 27.170 | 1.00 39.62 | 0 |
| ATOM | 2754 | 0 | | W5034 | | -22.175 | 28.942 | 1.00 33.59 | 0 |
| ATOM | 2755 | 0 | | W5035 | 7.766 | 9.184 | 29.149 | 1.00 37.38 | 0 |
| MOTA | 2756 | 0 | HOH | W5036 | 27.081 | 7.365 | 5.947 | 1.00 37.77 | 0 |

| ATOM | 2757 | 0 | HOH | W5037 | 26.538 | 19.381 | 35.080 | 1.00 37.77 | 0 |
|------|------|---|-----|-------|----------------|-----------------|-----------------|------------|-----|
| ATOM | 2758 | 0 | HOH | W5038 | -4.201 | 17.799 | 6.607 | 1.00 32.96 | 0 |
| ATOM | 2759 | 0 | HOH | W5039 | 5.036 | 8.700 | 14.260 | 1.00 30.11 | . 0 |
| MOTA | 2760 | 0 | нон | W5040 | 0.851 | 9.642 | 42.538 | 1.00 22.98 | 0 |
| MOTA | 2761 | 0 | HOH | W5041 | 19.927 | 0.231 | 15.198 | 1.00 20.70 | 0 |
| ATOM | 2762 | 0 | нон | W5042 | 38.613 | -9.206 | 13.685 | 1.00 46.18 | 0 |
| ATOM | 2763 | 0 | нон | W5043 | 35.672 | -15.638 | 5.122 | 1.00 43.16 | 0 |
| ATOM | 2764 | 0 | нон | W5044 | 14.774 | -8.966 | 39.562 | 1.00 27.43 | 0 |
| ATOM | 2765 | 0 | нон | W5045 | -0.343 | -11.294 | 8.886 | 1.00 35.83 | 0 |
| ATOM | 2766 | ō | | W5046 | 0.384 | 7.133 | 40.132 | 1.00 36.11 | 0 |
| ATOM | 2767 | o | | W5047 | | -16.597 | 10.364 | 1.00 51.74 | 0 |
| MOTA | 2768 | ō | | W5048 | 17.913 | 8.434 | 22.684 | 1.00 19.14 | 0 |
| ATOM | 2769 | ō | | W5049 | 26.849 | 7.812 | 30.849 | 1.00 32.50 | 0 |
| ATOM | 2770 | ō | | W5050 | 31.682 | 10.495 | 7.280 | 1.00 43.96 | 0 |
| ATOM | 2771 | ŏ | | W5051 | 33.295 | 7.550 | 31.842 | 1.00 42.65 | 0 |
| ATOM | 2772 | Ö | | W5052 | 26.726 | 22.667 | 9.308 | 1.00 42.17 | 0 |
| ATOM | 2773 | Ö | | W5053 | 16.839 | 2.653 | 43.220 | 1.00 32.73 | Ō |
| ATOM | 2774 | ŏ | | W5054 | 28.300 | 3.705 | 0.074 | 1.00 31.84 | Ō |
| ATOM | 2775 | ŏ | | W5055 | 21.249 | 10.241 | 40.281 | 1.00 40.01 | Ō |
| MOTA | 2776 | Ö | | W5056 | 18.910 | 0.164 | 43.189 | 1.00 35.91 | ŏ |
| ATOM | 2777 | Ö | | W5057 | 14.293 | 25.027 | 1.495 | 1.00 30.20 | Ö |
| ATOM | 2778 | Ö | | W5058 | 15.432 | -0.416 | 17.518 | 1.00 26.65 | Ö |
| ATOM | 2779 | 0 | | W5059 | 21.028 | 5.383 | 41.219 | 1.00 20.03 | 0 |
| | - | | | W5059 | 27.025 | 7.703 | 33.714 | 1.00 31.00 | 0 |
| ATOM | 2780 | 0 | | | | -2.470 | 38.136 | 1.00 38.38 | 0 |
| ATOM | 2781 | 0 | | W5061 | 1.162 7.118 | -4.468 | 3.111 | 1.00 32.76 | 0 |
| ATOM | 2782 | 0 | | W5062 | 10.345 | | 50.558 | 1.00 23.42 | 0 |
| ATOM | 2783 | 0 | | W5063 | | 8.046 -6.957 | | 1.00 21.47 | 0 |
| ATOM | 2784 | 0 | | W5064 | 1.601 | | 7.392 48.256 | | 0 |
| MOTA | 2785 | 0 | | W5065 | 8.301 | • | | 1.00 31.31 | 0 |
| ATOM | 2786 | 0 | | W5066 | 13.857 | 7.152 | 1.988 | 1.00 29.65 | 0 |
| ATOM | 2787 | 0 | | W5067 | -8.101 | -4.494 | | 1.00 34.47 | 0 |
| ATOM | 2788 | 0 | | W5068 | | -17.405 | 6.589 | 1.00 41.64 | 0 |
| ATOM | 2789 | 0 | | W5069 | | -25.606 | 27.581 | 1.00 27.36 | 0 |
| ATOM | 2790 | 0 | | W5070 | 23,222 | 14.650 | 26.416 | 1.00 26.05 | 0 |
| ATOM | 2791 | 0 | | W5071 | 7.588 | -0.528 | 0.314 | 1.00 32.42 | |
| ATOM | 2792 | 0 | | W5072 | | -17.275 | 4.444 | 1.00 27.98 | 0 |
| ATOM | 2793 | 0 | | W5073 | | -13.814 | 28.837 | 1.00 53.93 | . 0 |
| MOTA | 2794 | 0 | | W5074 | 32.339 | 6.763 | 6.234 | 1.00 44.01 | 0 |
| MOTA | 2795 | 0 | | W5075 | | -21.822 | 12.391 | 1.00 27.13 | |
| ATOM | 2796 | 0 | | W5076 | 2.962 | 14.623 | 32.943 | 1.00 35.34 | 0 |
| ATOM | 2797 | 0 | | W5077 | | -11.144 | 17.921 | 1.00 32.13 | |
| MOTA | 2798 | 0 | | W5078 | 21.073 | 24.057 | -0.096 | | 0, |
| ATOM | 2799 | 0 | | W5079 | | -12.595 | 24.369 | 1.00 37.81 | ` 0 |
| ATOM | 2800 | 0 | | W5080 | 26.131 | 21.190 | 0.182 | 1.00 31.04 | 0 |
| ATOM | 2801 | 0 | | W5081 | -7.427 | -1.162 | 30.153 | 1.00 37.22 | |
| ATOM | 2802 | 0 | | W5082 | 9.376 | 19.648 | 13.353 | 1.00 46.89 | 0 |
| ATOM | 2803 | 0 | | W5083 | | -14.783 | 26.158 | 1.00 30.66 | 0 |
| MOTA | 2804 | 0 | | W5085 | 24.158 | -4.023 | 38.598 | 1.00 29.95 | |
| ATOM | 2805 | 0 | | W5086 | 2.673 | ~2.236 | 40.838 | 1.00 36.71 | 0 |
| ATOM | 2806 | 0 | | W5087 | 14.901 | 15.719 | 31.793 | 1.00 66.05 | 0 |
| MOTA | 2807 | 0 | | W5089 | 0.185 | 6.149 | 5.302 | 1.00 45.92 | 0 |
| MOTA | 2808 | 0 | | W5090 | -3.050 | 13.963 | 3.439 | 1.00 31.57 | 0 |
| ATOM | 2809 | 0 | | W5091 | 20.002 | 26.238 | 4.307 | 1.00 38.95 | 0 |
| ATOM | 2810 | 0 | | W5092 | 9.528 | 7.010 | 25.049 | 1.00 40.00 | 0 |
| ATOM | 2811 | 0 | | W5093 | 22.998 | 9.245 | 25.495 | 1.00 45.96 | 0 |
| MOTA | 2812 | 0 | | W5094 | 25.633 | | 41.203 | 1.00 33.74 | 0 |
| MOTA | 2813 | 0 | нон | W5095 | 22.525 | 7.413 | 40.125 | 1.00 27.93 | 0 |

| ATOM | 2814 | 0 | нон | W5096 | 25.772 | -0.812 | 38.637 | 1.00 43.16 | | 0 |
|-------|------|---|------|---------|--------|---------|--------|------------|---|---|
| ATOM | 2815 | 0 | нон | W5097 | 1.675 | 3.923 | 15.398 | 1.00 24.93 | | 0 |
| ATOM | 2816 | 0 | нон | W5098 | 3.426 | 25.166 | 2.688 | 1.00 33.60 | | 0 |
| ATOM | 2817 | 0 | нон | W5099 | 6.716 | 24.079 | 2.431 | 1.00 30.61 | | 0 |
| ATOM | 2818 | 0 | нон | W5100 | 13.776 | 2.826 | 15.316 | 1.00 35.09 | | 0 |
| ATOM | 2819 | 0 | нон | W5101 | 2.840 | 22.627 | 5.321 | 1.00 28.88 | | 0 |
| ATOM: | 2820 | 0 | HOH- | W5102 | 4.306 | 26.695 | 0.803 | 1.00 45.75 | | 0 |
| MOTA | 2821 | 0 | нон | W5103 | 28.312 | 3.533 | 30.225 | 1.00 30.56 | | 0 |
| MOTA | 2822 | 0 | нон | W5104 | 7.296 | 5.105 | 45.493 | 1.00 44.55 | | 0 |
| MOTA | 2823 | 0 | HOH | W5105 | 8.727 | -7.822 | 20.152 | 1.00 30.96 | | 0 |
| ATOM | 2824 | 0 | нон | W5106 | 15.910 | 2.991 | 1.288 | 1.00 26.19 | | 0 |
| MOTA | 2825 | 0 | нон | W5107 | 24.692 | 15.648 | 32.485 | 1.00 45.46 | | 0 |
| MOTA | 2826 | 0 | нон | W5108 | 10.229 | 10.752 | 16.032 | 1.00 39.52 | | 0 |
| ATOM | 2827 | 0 | НОН | W5109 | 30.124 | 8.492 | 1.194 | 1.00 42.53 | | 0 |
| MOTA | 2828 | 0 | нон | W5110 | 38.431 | 9.460 | 12.406 | 1.00 34.79 | | 0 |
| MOTA | 2829 | 0 | нон | W5111 | 15.296 | -0.704 | 44.230 | 1.00 30.31 | | 0 |
| ATOM | 2830 | 0 | НОН | W5112 | 22.219 | -25.058 | 0.518 | 1.00 40.16 | | 0 |
| ATOM | 2831 | 0 | НОН | W5113 | 16.280 | -1.757 | 13.031 | 1.00 32.98 | | 0 |
| ATOM | 2832 | 0 | НОН | W5114 | 7.672 | 5.118 | 50.500 | 1.00 42.44 | | 0 |
| MOTA | 2833 | 0 | нон | W5116 | 19.588 | 26.165 | 1.692 | 1.00 35.11 | | 0 |
| MOTA | 2834 | 0 | нон | W5117 | 29.689 | 0.468 | 33.170 | 1.00 50.63 | | 0 |
| MOTA | 2835 | 0 | HOH | W5118 | 27.638 | 14.621 | 27.167 | 1.00 37.33 | | 0 |
| ATOM | 2836 | 0 | нон | W5119 | 25.674 | 24.122 | 6.832 | 1.00 44.26 | | 0 |
| ATOM | 2837 | 0 | НОН | W5120 | 40.801 | -13.288 | 5.322 | 1.00 31.98 | | 0 |
| ATOM | 2838 | 0 | нон | W5121 | 36.143 | -1.829 | 16.148 | 1.00 41.24 | | 0 |
| MOTA | 2839 | 0 | нон | W5122 | 3.151 | 5.682 | 48.883 | 1.00 34.36 | | 0 |
| ATOM | 2840 | 0 | нон | W5123 | 32.693 | 14.445 | 9.290 | 1.00 34.74 | | 0 |
| MOTA | 2841 | 0 | НОН | W5124 | 28.701 | 6.185 | 34.708 | 1.00 49.77 | | 0 |
| MOTA | 2842 | 0 | нон | W5125 | 26.196 | 1.517 | -1.280 | 1.00 39.43 | | 0 |
| MOTA | 2843 | 0 | нон | W5126 | -0.033 | 0.726 | 10.398 | 1.00 47.62 | | 0 |
| MOTA | 2844 | Ō | нон | W5127 | 21.383 | -3.597 | -1.922 | 1.00 51.56 | | 0 |
| ATOM | 2845 | 0 | нон | W5128 - | 13.364 | 12.833 | 27.633 | 1.00 52.29 | | 0 |
| MOTA | 2846 | 0 | нон | W5129 | 21.714 | 12.615 | 35.721 | 1.00 33.09 | | 0 |
| MOTA | 2847 | 0 | нон | W5130 | 8.469 | 6.895 | 52.440 | 1.00 45.76 | | 0 |
| MOTA | 2848 | 0 | нон | W5131 | 26.110 | 4.660 | 30.832 | 1.00 35.30 | | 0 |
| MOTA | 2849 | 0 | нон | W5132 | 19.463 | -23.363 | 14.165 | 1.00 35.76 | | 0 |
| ATOM | 2850 | 0 | нон | W5133 | 13.443 | 20.073 | -9.252 | 1.00 40.04 | | 0 |
| MOTA | 2851 | 0 | нон | W5134 | 9.131 | 8.743 | 16.901 | 1.00 44.35 | | 0 |
| MOTA | 2852 | 0 | нон | W5135 | 2.141 | 8.144 | 15.984 | 1.00 43.82 | * | 0 |
| MOTA | 2853 | 0 | нон | W5136 | 8.533 | 27.824 | 6.026 | 1.00 33.71 | | 0 |
| ATOM | 2854 | 0 | нон | W5137 | 23.489 | 23.402 | 0.284 | 1.00 47.94 | | 0 |
| MOTA | 2855 | 0 | нон | W5138 | 19.996 | 15.564 | -7.451 | 1.00 42.23 | | 0 |
| MOTA | 2856 | 0 | НОН | W5139 | 3.830 | 6.820 | -6.454 | 1.00 43.70 | | 0 |
| MOTA | 2857 | 0 | | W5140 | 15.282 | 15.611 | 18.402 | 1.00 41.11 | | 0 |
| ATOM | 2858 | 0 | | W5141 | 17.265 | 26.061 | 11.713 | 1.00 39.14 | | 0 |
| MOTA | 2859 | 0 | | W5142 | 23.754 | 1.893 | -2.493 | 1.00 45.81 | | 0 |
| MOTA | 2860 | 0 | | W5143 | 26.488 | 3.338 | 6.608 | 1.00 42.72 | | 0 |
| ATOM | 2861 | 0 | | W5144 | 6.963 | | 1.634 | 1.00 33.11 | | 0 |
| MOTA | 2862 | 0 | | W5145 | -0.293 | | 3.517 | 1.00 47.82 | | 0 |
| ATOM | 2863 | 0 | | W5146 | 13.304 | | 14.071 | 1.00 44.49 | | 0 |
| ATOM | 2864 | 0 | | W5147 | 14.485 | | 11.196 | 1.00 34.10 | | 0 |
| ATOM | 2865 | 0 | | W5148 | 38.684 | | 16.424 | 1.00 42.58 | | 0 |
| ATOM | 2866 | 0 | | W5149 | -0.378 | | 41.179 | 1.00 39.92 | | 0 |
| ATOM | 2867 | 0 | | W5150 | 14.999 | | 38.087 | 1.00 56.40 | | 0 |
| ATOM | 2868 | 0 | | W5151 | | -10.394 | 33.773 | 1.00 51.57 | | 0 |
| MOTA | 2869 | 0 | | W5152 | 9.035 | | 0.106 | 1.00 46.37 | | 0 |
| ATOM | 2870 | 0 | HOH | W5153 | 5.110 | -2.372 | 2.316 | 1.00 33.68 | | 0 |

| ATOM | 2871 | 0 | НОН | W5154 | 29.018 | -14.387 | 13.400 | 1.00 40.14 | Ò |
|------|------|-----|-----|-------|--------|---------|--------|------------|-----|
| MOTA | 2872 | 0 | нон | W5155 | 1.676 | -2.447 | 9.577 | 1.00 41.85 | 0.0 |
| ATOM | 2873 | 0 | нон | W5156 | 20.185 | 11.538 | -6.635 | 1.00 37.49 | 0 |
| MOTA | 2874 | 0 | | W5157 | | -28.857 | 26.962 | 1.00 41.90 | 0 |
| ATOM | 2875 | 0 | | W5158 | -6.106 | 19.784 | 6.635 | 1.00 36.72 | 0 |
| ATOM | 2876 | Ō | | W5159 | 5.517 | 17.184 | 13.233 | 1.00 48.23 | 0 |
| MOTA | 2877 | ŏ | | W5160 | 5.076 | 15.020 | 11.985 | 1.00 45.45 | Ō |
| ATOM | 2878 | 0 | | W5161 | 5.445 | -7.849 | 27.659 | 1.00 39.11 | Ō |
| ATOM | 2879 | 0 | | W5162 | 20.980 | 18.101 | 37.922 | 1.00 29.42 | Ō |
| ATOM | 2880 | 0 | | W5163 | | -29.146 | 3.293 | 1.00 42.39 | Ö |
| ATOM | 2881 | 0 | | W5164 | 30.770 | 4.871 | 31.188 | 1.00 43.36 | 0 |
| ATOM | 2882 | | | W5165 | 3.854 | -8.929 | 29.337 | 1.00 54.81 | . 0 |
| | | 0 | | W5166 | 10.593 | 19.605 | 16.042 | 1.00 47.04 | Ö |
| ATOM | 2883 | 0 | | | 42.095 | 8.840 | 19.150 | 1.00 47.64 | 0 |
| ATOM | 2884 | 0 | | W5167 | | 11.390 | | 1.00 42.37 | 0 |
| MOTA | 2885 | 0 | | W5168 | 9.957 | | 13.550 | | |
| ATOM | 2886 | 0 | | W5169 | -4.606 | 21.333 | 1.399 | 1.00 48.40 | 0 |
| MOTA | 2887 | 0 | | W5170 | 11.695 | 29.342 | 6.480 | 1.00 58.15 | 0 |
| ATOM | 2888 | 0 | | W5171 | 23.099 | 25.128 | 3.657 | 1.00 40.99 | 0 |
| MOTA | 2889 | 0 | | W5172 | 23.505 | 24.766 | -3.702 | 1.00 44.31 | 0 |
| ATOM | 2890 | 0 | | W5173 | 14.447 | 17.461 | 20.573 | 1.00 40.93 | 0 |
| ATOM | 2891 | 0 | | W5174 | 11.974 | 23.606 | 15.698 | 1.00 50.59 | 0 |
| ATOM | 2892 | 0 | | W5175 | 33.868 | 19.345 | 11.374 | 1.00 39.71 | 0 |
| ATOM | 2893 | 0 | | W5176 | 8.306 | -9.142 | 31.222 | 1.00 42.33 | 0 |
| ATOM | 2894 | 0 | | W5177 | 12.171 | 14.379 | 29.266 | 1.00 52.75 | 0 |
| MOTA | 2895 | , 0 | | W5178 | 29.974 | -2.958 | 37.157 | 1.00 38.64 | 0 |
| MOTA | 2896 | 0 | нон | W5179 | 30.177 | 1.102 | 3.621 | 1.00 43.39 | 0 |
| ATOM | 2897 | 0 | HOH | W5180 | 13.634 | | 1.980 | 1.00 43.54 | 0 |
| MOTA | 2898 | 0 | | W5181 | 9.893 | | 25.719 | 1.00 35.63 | 0 |
| MOTA | 2899 | 0 | | W5182 | 15.133 | 16.851 | 24.775 | 1.00 34.15 | 0 |
| TER | 2900 | | HOH | W5182 | | | | | |
| MOTA | 2901 | NIA | COE | E4002 | 19.788 | -13.382 | 22.863 | 1.00 37.66 | N |
| MOTA | 2902 | C2A | COE | E4002 | 19.629 | -12.509 | 21.832 | 1.00 37.59 | С |
| MOTA | 2903 | AEN | COE | E4002 | 18.590 | -12.603 | 20.980 | 1.00 37.39 | N |
| MOTA | 2904 | C4A | COE | E4002 | 17.686 | -13.627 | 21.196 | 1.00 37.85 | С |
| ATOM | 2905 | C5A | COE | E4002 | | -14.571 | 22.262 | 1.00 38.04 | C |
| MOTA | 2906 | C6A | COE | E4002 | 18.900 | -14.393 | 23.079 | 1.00 38.11 | C |
| ATOM | 2907 | N6A | COE | E4002 | 19.128 | -15.221 | 24.120 | 1.00 38.32 | N |
| MOTA | 2908 | N7A | COE | E4002 | 16.749 | -15.454 | 22.198 | 1.00 38.10 | N |
| MOTA | 2909 | C8A | COE | E4002 | | -15.090 | 21.125 | 1.00 38.02 | С |
| ATOM | 2910 | N9A | COE | E4002 | | -13.990 | 20.508 | 1.00 38.30 | N |
| ATOM | 2911 | C71 | COE | E4002 | | -13.354 | 19.309 | 1.00 38.56 | C |
| ATOM | 2912 | C72 | COE | E4002 | 15.686 | -14.244 | 18.059 | 1.00 38.64 | C |
| ATOM | 2913 | 072 | COE | E4002 | 16.358 | -13.703 | 16.916 | 1.00 37.72 | 0 |
| MOTA | 2914 | C73 | COE | E4002 | 14.168 | -14.225 | 17.883 | 1.00 39.06 | С |
| MOTA | 2915 | 073 | COE | E4002 | 13.797 | 14.451 | 16.455 | 1.00 38.84 | 0 |
| MOTA | 2916 | P73 | COE | E4002 | 14.041 | -15.822 | 15.721 | 1.00 39.24 | P |
| MOTA | 2917 | 07A | COE | E4002 | 13.165 | -15:826 | 14.433 | 1.00 39.04 | 0 |
| ATOM | 2918 | A80 | COE | E4002 | 15.540 | -15.939 | 15.325 | 1.00 39.12 | 0 |
| MOTA | 2919 | 09A | COE | E4002 | 13.637 | -17.009 | 16.646 | 1.00 39.35 | 0 |
| ATOM | 2920 | C74 | COE | E4002 | | -12.831 | 18.392 | 1.00 39.77 | С |
| ATOM | 2921 | | | E4002 | | -12.631 | 19.516 | 1.00 39.23 | 0 |
| ATOM | 2922 | | | E4002 | | -12.657 | 18.817 | 1.00 40.70 | C |
| ATOM | 2923 | | | E4002 | 12.121 | -11.261 | 19.226 | 1.00 42.75 | 0 |
| ATOM | 2924 | | | E4002 | | -10.752 | 19.901 | 1.00 43.64 | P |
| ATOM | 2925 | | | E4002 | | -11.915 | 20.051 | 1.00 43.83 | 0 |
| ATOM | 2926 | | | E4002 | 10.208 | | 19.036 | 1.00 44.05 | 0 |
| ATOM | 2927 | | | E4002 | | -10.230 | 21.306 | 1.00 43.87 | 0 |
| | | | | | | | | | |

TER 2928 COE E4002 END 1